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MONTE CARLO DETERMINATION OF THE CHARACTERISTIC LIMITS IN MEASUREMENT OF IONISING RADIATION—FUNDAMENTALS AND NUMERICS

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It is shown how the decision threshold, the detection limit and the limits of a coverage interval — summarily called the characteristic limits — and, in addition, the best estimate and the associated standard uncertainty of a non-negative radiation measurand are to be calculated by using the Monte Carlo (MC) method in ionising-radiation measurements. The limits are mathematically defined by means of quantiles of the Bayesian distributions of the possible measurand values. The MC-induced uncertainties of the limits and typical problems connected with MC application are also treated. The paper can serve as a bridge between the ISO *Guide to the Expression of Uncertainty in Measurement* (GUM), Supplement 1 applying the MC method and ISO/FDIS 11929 (at present in preparation) dealing with the characteristic limits. As an illustration, a net count rate measurand, being the difference of a gross and a background count rate, is treated theoretically and numerically. More complex examples deal with the wipe test for surface contamination and with a linear multi-channel spectrum unfolding.

INTRODUCTION

The recognition and detection of ionising radiation are indispensable basic prerequisites for radiation protection. For this purpose, the standard series ISO 11929 provides *characteristic limits*, i.e. the decision threshold, the detection limit and the confidence limits, for a diversity of application fields. The *decision threshold* allows a decision to be made for a measurement on whether or not, for instance, radiation of a possibly radioactive sample is present. The *detection limit* allows a decision to be made on whether or not the measurement procedure intended for application to the measurement meets the requirements to be fulfilled and is, therefore, appropriate for the measurement purpose. *Confidence limits* — recently called the *limits of a coverage interval*, also in the present paper — enclose with a specified probability the *true value* of the *measurand*, the physical quantity to be measured. In addition, the *best estimate* of the measurand and the associated *standard uncertainty* are of interest, together as the *measurement result*.

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Because of recent developments in metrology concerning measurement uncertainty, laid down in the ISO *Guide to the Expression of Uncertainty in Measurement* (GUM)[1], the standard series ISO 11929 urgently needs revision. Therefore, a new draft ISO/FDIS 11929[2] has been elaborated by the authors of the present paper and others on the basis of GUM, but using *Bayesian statistics* (BS)[3–12] and the Bayesian theory of measurement uncertainty[14–16]. This theory provides the Bayesian foundation of GUM. Moreover, the draft (2) is based on the definitions of the characteristic limits[17], the standard proposal[18], the introducing article[19] and the precursory ISO 11929-7[20]. It unifies and should replace the old parts of ISO 11929 and will be applicable not only to a large variety of particular measurements of ionising radiation but also, in analogy, to other measurement procedures.

Meanwhile, a supplement[21] to GUM[1] has been published, dealing comprehensively with the treatment of measurement uncertainty using the Monte Carlo (MC) method in complex measurement evaluations. This gave the incentive for writing the present paper, which is intended to be taken as the corresponding supplement to ISO/FDIS 11929[2].

The paper is also essentially founded on BS and will serve as a bridge between documents[2,21].

The MC methods provided by the GUM supplement[21] and by the present paper should not only be applied in complex cases but also in simpler cases — such as the wipe test (see Appendix 3) — where only some few input quantities using non-Gaussian distributions or strongly non-linear model equations are involved. Moreover, these MC methods can be used for independently testing whether or not the methods offered by GUM and ISO/FDIS 11929 are sufficient for the particular measurements in question, for instance, in low-level measurements. However, the MC methods do not always have to be applied because of the *central limit theorem* of probability theory. This theorem states that the measurand can in most cases be assessed, at least approximately, by using a Gaussian normal distribution if the measurand depends sufficiently linearly on several input quantities in the data region of interest. The parameters of the Gaussian distribution can be obtained already by the methods provided by GUM. More details are given in the following.

Applying BS together with the *principle of maximum (information) entropy* (PME)[10–15] in the present paper makes it possible to take also into account non-statistical information, for instance, of uncertain physical quantities and influences, which do not behave randomly in repeated or counting measurements and thus cannot be treated by conventional, frequency-based statistics (CS). BS and CS are both based on the probability theory but differ essentially in their understanding of the probability $\Pr(A)$ of a random event A. In CS, the probability is the limit of the relative frequency with which the event happens randomly in measurements repeated independently more and more frequently under identical nominal conditions. In contrast, the probability in BS expresses the degree of belief, based on the information actually available, that the event will happen in a measurement *before* the measurement is carried out. An example is the probability $1/2$ reasonably assigned to each side of a coin before tossing the coin. This meaning of probability is in fact the classical one introduced by Bernoulli and Laplace. BS and CS are asymptotically equivalent on the same base of data, conditions, assumptions and other information if both statistics are applicable. For a comprehensive comparison of BS and CS in repeated measurements, see Lira and Wöger[22].

There are two quite distinct statistical levels when MC is applied to determine the characteristic limits. They should be strictly separated in mind. On the one hand, there is a metrological level where measurement data and other information are evaluated statistically and probability-based statements are obtained on the measurand, including those on uncertainty and the characteristic limits. Here, BS has to be used because non-randomly behaving quantities cannot be treated by CS. On the other hand, there is a MC level. The MC method as applied in the supplement[21] and in the present paper merely serves as a convenient tool for more easily calculating complex integrals numerically, but can never change the Bayesian understanding of a probability distribution. The MC sampling does not simulate any repeated measurements, although it appears similar to them with an arbitrarily large number of repetitions and without non-random influences. Either BS or CS can therefore be applied on the MC level, but strictly separated from all the Bayesian interpretations, otherwise on the metrological level.

The present paper is written mainly for experts, tutors and developers of procedures and programs in the fields of characteristic limits and MC. The aims and basic tools of the study are stated in the following two sections. Several probability distributions are first formally introduced. In particular, these are distributions of the measurand Y, which depends by a *model equation* $Y = G(X_1, X_2, \ldots)$ on *input quantities* X_i, with their joint distribution also needed to perform a *distribution propagation* from X_i to Y. Then the best estimate of the measurand with the associated standard uncertainy and the characteristic limits to be determined are defined by means of integrals, i.e. moments and quantiles, of the distributions of Y. The way to establish distributions in general from available information by using the PME or other methods such as the Bayes theorem is shown in a further section. The point of view is then changed from the metrological level to the MC level in order to apply the MC method. The next two sections describe how to draw MC samples from the distributions and how to calculate the integrals by MC. The last section and, more deeply, Appendix 4 deal with the MC-induced uncertainty of the integral calculation. As an illustration, a counting measurement and a linear spectrum unfolding are treated theoretically in Appendix 1 as typical, still relatively simple examples of ionising-radiation measurements. Numerical results obtained by the Gaussian approach according to ISO/FDIS 11929[2] and by the analytical and MC approaches to the counting measurement and to the wipe test are compared in Appendices 2 and 3, respectively. Typical problems involved in the MC application are also treated in Appendix 3.

For the definitions of the metrological terms used, see references (1,2,21,23), and for the statistical terms and symbols, see, e.g. references (24–26). There are problems in this respect between BS and CS, between BS with and without PME and in nomenclature and notation. To avoid misunderstandings in

such cases, it is tried, if necessary, to clearly and exactly define the concepts in question where they are introduced and to call and denote them as closely to other usages as suitable and possible. A glossary of some important terms and symbols is given in Appendix 5.

DISTRIBUTIONS

Denotations

In the following if not otherwise stated, an upper-case letter, say Z, is used to denote some random variable and (preferably corresponding) lower-case letters z or ζ are used for values of the random variable. The distinct meanings of the random variable and its values should always be kept in mind. Boldface symbols are used for sets of related entities. For instance, a set of quantities or values $\{v_1, v_2, \ldots\}$ is abbreviated by the corresponding symbol $\mathbf{v}$ used as a column matrix $(v_1, v_2, \ldots)^\top$. The due $\mathbf{v}$-space volume element $\mathrm{d}\mathbf{v}$ is applied in multiple integrals. The probability density, also called the *distribution*, of a random variable Z is denoted by $f_Z(z \mid \mathbf{a})$ (similarly to DIN 13303-1[25]) and to the symbol $\{z \mid \mathbf{a}\}$ for a set of elements z with a property described by $\mathbf{a}$). The set $\mathbf{a}$ summarily represents all the information taken into account, i.e. data, conditions, assumptions, functional relations and other relevant information given or obtained from measurements and other sources. The data can also comprise values of other random variables as statistical information, e.g. in the form $V = v$ or, shorter, v alone for a random variable V with its value v. Other information may be non-statistical such as functional relations. Particular fixed values of a random variable are marked by suitable affixes. As in common practice and in ISO/FDIS 11929[2], the general symbol f is used for probability densities and F for the corresponding *distribution functions*, for instance, $F_Z(z \mid \mathbf{a}) = \Pr(Z \le z \mid \mathbf{a}) = \int_{-\infty}^{z} f_Z(\zeta \mid \mathbf{a})\mathrm{d}\zeta$ or, conversely, $f_Z(z \mid \mathbf{a}) = \mathrm{d}F_Z(z \mid \mathbf{a})/\mathrm{d}z$. The joint distribution of a set $\mathbf{Z}$ of random variables Z_i with values $\mathbf{z}$ is denoted by $f_{\mathbf{Z}}(\mathbf{z} \mid \mathbf{a})$. Instead of f and F, the symbols g and G, respectively, are used in the GUM supplement[21]. Notice that the random variable as a subscript of the distribution symbols f and F is not dropped[25]. This avoids mistakes, which can be caused easily by the less informative, but simpler, naked symbols usually preferred in the literature.

A random variable Z, called an *estimator*, is assigned to every particular physical quantity involved. Its values z (or ζ) are *estimates* of the physical quantity. Only for brevity and convenience, the quantity and its estimator are denoted by the same symbol Z if suitable and not otherwise stated, although they are not identical and should be distinguished as physical and mathematical entities, respectively. In this way, for instance, 'estimator R of the count rate' can be shortened to 'count rate R', although the count rate is not a random variable if the count rate is taken as a physical quantity with a fixed *true value* to be determined.

The distribution $f = f_Z(z \mid \mathbf{a})$ of the estimator Z represents the probability of an estimate z to be the true value of the physical quantity on the information $\mathbf{a}$. The estimate z is therefore also taken as a *possible true value* if $f > 0$. An already known or assumed f used as a computation input is called a *prior*. It is stressed again that in BS applied here on the metrological level, a distribution such as f in most cases is a probability density in a degree-of-belief sense and represents the information about the physical quantity actually being present and taken into account. Such a distribution is not that of values which occur in measurements repeated many times under identical or similar nominal conditions as in CS. However, CS frequency distributions may also be involved, for instance, the Poisson distribution in counting measurements.

Distribution propagation

Estimator sets $\mathbf{X}$ and $\mathbf{Y}$ of the involved physical *input* and *output quantities* are considered with values $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$, respectively. Their joint distributions based on information sets $\mathbf{a}$ and $\mathbf{a}'$, respectively, meet the product rule

$$f_{\mathbf{X},\mathbf{Y}}(\boldsymbol{\xi}, \boldsymbol{\eta} \mid \mathbf{a}, \mathbf{a}') = f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{X} = \boldsymbol{\xi}, \mathbf{a}') f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) \tag{1}$$

This rule follows from the general probability product rule $\Pr(A \cap B) = \Pr(A \mid B)\Pr(B)$ for random events (sets) A and B. In many cases, the set $\mathbf{a}$ mainly contains the input data information and the set $\mathbf{a}'$ the relations between $\mathbf{X}$ and $\mathbf{Y}$, i.e. the model information, and further, updating data. The first distribution on the right-hand side of equation (1) is therefore sometimes called the *model prior* and the second one the *(data) prior* or *input distribution*, although the different kinds of information cannot always be strictly separated. The *output distribution* of $\mathbf{Y}$, also called the *posterior*, on the combined information $\mathbf{a},\mathbf{a}'$ is the distribution of very interest. It is obtained from equation (1) by a *maginalisation*:

$$\begin{aligned} f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{a}, \mathbf{a}') &= \int f_{\mathbf{X},\mathbf{Y}}(\boldsymbol{\xi}, \boldsymbol{\eta} \mid \mathbf{a}, \mathbf{a}')\mathrm{d}\boldsymbol{\xi} \\ &= \int f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{X} = \boldsymbol{\xi}, \mathbf{a}') f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})\mathrm{d}\boldsymbol{\xi} \end{aligned} \tag{2}$$

Some important formulas needed are derived in the following from the posterior by application, together with equation (1), to some particular model

priors $f_{\mathbf{Y}}(\boldsymbol{\eta} \mid \mathbf{X} = \boldsymbol{\xi}, \mathbf{a}')$ in the integrand. These distributions represent the *model relations*, which form $\mathbf{a}'$ and have to be observed between the involved physical quantities (and the corresponding estimators). Model relations $M_i(\mathbf{X}, \mathbf{Y}) = 0$ or ≥ 0 are considered. They may depend also on data contained in the information sets. The model priors are expressed by $C_i\delta(M_i)$ for $M_i(\boldsymbol{\xi}, \boldsymbol{\eta}) = 0$ or $C_i H(M_i)$ for $M_i \geq 0$ with suitable constants C_i. If there are several model relations to be observed in a particular case, then the corresponding priors must be multiplied to form the total model prior. The considered priors are based on the Heaviside unit step function $H(t) = 1$ $(t \geq 0)$ and $H(t) = 0$ $(t < 0)$. Its derivative $\delta(t) = \mathrm{d}H(t)/\mathrm{d}t$ is called the Dirac delta function. It has the properties $\delta(t) = 0$ $(t \neq 0)$ and $\int_{-\infty}^{\infty} \delta(t) g(t) \mathrm{d}t = g(0)$ for any function $g(t)$.

In order to define the characteristic limits in measurements of ionising radiation, a non-negative particular physical quantity Y, called the *measurand*, is considered that quantifies the radiation effect of interest and assumes the true value 0 if the effect is not present. This measurand is the very quantity for which the true value and the characteristic limits are to be determined. An estimator, also denoted by Y, with values y (or η) is assigned to the measurand.

The measurand Y depends on several input quantities $\mathbf{X}$. This is expressed by the model equation $M = Y - G(\mathbf{X}) = 0$ or $Y = G(\mathbf{X})$. The input distribution $f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$ together with the model prior $f_Y(y \mid \mathbf{X} = \boldsymbol{\xi}, y = G(\boldsymbol{\xi})) = C\,\delta(y - G(\boldsymbol{\xi}))$, where the information $\mathbf{a}'$ is formed by the relation $y = G(\boldsymbol{\xi})$, then yields according to equations (1) and (2) the posterior

$$\begin{aligned} f_Y(y \mid \mathbf{a}) &= \int \delta(y - G(\boldsymbol{\xi})) f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) \mathrm{d}\boldsymbol{\xi}; \\ F_Y(y \mid \mathbf{a}) &= \int H(y - G(\boldsymbol{\xi})) f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) \mathrm{d}\boldsymbol{\xi} \end{aligned} \tag{3}$$

$C = 1$ is obtained by normalisation. The model function G may also depend on the information $\mathbf{a}$, for instance, on the uncertainties involved in spectrum unfolding (see Appendix 1). Instead of G, the symbol f is used in GUM[1,21]. In many cases, the posterior $f_Y(y \mid \mathbf{a})$ turns out to be at least approximately a Gaussian normal distribution. Equation (3) is called the *Markov formula*. It is the well-known, basic equation of *distribution propagation*[21] or transformation from $\mathbf{X}$ to Y in the probability theory.

Particular estimates y of the measurand Y may be negative when obtained from measurement data or generated by MC, but only the estimates $y \geq 0$ are possible true values of the non-negative measurand. This knowledge is in most cases not taken into account in $\mathbf{a}$ and, thus, requires an update. This is done by introducing the additional model relation $M' = Y \geq 0$ and the corresponding model prior $f_Y(y \mid y \geq 0) = C\ H(y)$, which has to be multiplied with the delta function in equation (3) to form the total model prior. But $H(y)$ does not depend on $\boldsymbol{\xi}$ and can thus be drawn to the front of the integral. In this way, the posterior

$$\begin{aligned} f_Y(y \mid \mathbf{a}, y \geq 0) &= \frac{H(y) f_Y(y \mid \mathbf{a})}{I_0}; \\ I_0 &= \int_0^{\infty} f_Y(y \mid \mathbf{a}) \mathrm{d}y = 1 - F_Y(0 \mid \mathbf{a}) \end{aligned} \tag{4}$$

of the possible true measurand values on the combined information easily follows from equation (3). The normalisation constant $C = 1/I_0$ is obtained. See also the paragraph between equations (15) and (16) for a derivation of equation (4) from the PME.

Other formulas, which are better suited for MC application than equation (3), follow from equations (3) and (4), for example,

$$\begin{aligned} F_Y(y \mid \mathbf{a}, y \geq 0) &= \frac{1}{I_0} \int_{\mathbf{R}} f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) \mathrm{d}\boldsymbol{\xi}; \\ \mathbf{R} &= \{\boldsymbol{\xi} \mid 0 \leq G(\boldsymbol{\xi}) \leq y\}; \\ I_0 &= \int_{G(\boldsymbol{\xi}) \geq 0} f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) \mathrm{d}\boldsymbol{\xi}. \end{aligned} \tag{5}$$

Information modification

It may be asked why the condition $y \geq 0$ is not taken as included in the information set $\mathbf{a}$ from the beginning but is later added to form $f_Y(y \mid \mathbf{a}, y \geq 0)$. The reason is that $\mathbf{a}$ may contain a primary estimate y_0 of the measurand and the associated standard uncertainty $u(y_0)$, both obtained from an evaluation of measurements according to GUM[1] where the condition $y \geq 0$ is not taken into account and y_0 may become negative. Therefore, the condition must subsequently be observed. The model function G can be used to determine the primary estimate $y_0 = G(\mathbf{x}_0)$ from the available data $\mathbf{x}_0$ of the input quantities $\mathbf{X}$. A primary estimate y_0 is also needed for the decision on whether or not the radiation effect in question, quantified by the measurand, is recognised as present, for instance, the radiation of a measured, possibly radioactive sample. This decision has to be made by comparing y_0 with the decision threshold y^* (see the following section).

Unfortunately, not all the necessary elements of the set $\mathbf{a}$ are available in the situation where the decision threshold and the detection limit are to be determined. For instance, the result of a gross-effect radiation measurement is missing in this case, since

the decision threshold and the detection limit should be known before the first gross-effect measurement is carried out. A suitable true measurand value $\tilde{y} \geq 0$ is then assumed for an indirect compensation, and $\mathbf{a}$ is replaced by $\tilde{\mathbf{a}}(\tilde{y})$. This function transforms the present information for a chosen $\tilde{y}$. At least a reasonable approximation must be available, but it is not easy to establish this function in practice. The function $\tilde{\mathbf{a}}(\tilde{y})$ is a generalisation of the uncertainty function $\tilde{u}(\tilde{y})$ introduced in ISO/FDIS 11929[2]. If the gross-effect value, say x_1, of a radiation measurement is not available, y is replaced by $\tilde{y}$ in the model equation $y = G(\mathbf{x})$ and this equation is solved for x_1 resulting in $x_1 = L(\tilde{y}, x_2, \ldots)$, which is then used to form $\tilde{\mathbf{a}}(\tilde{y})$ and the distribution $f_Y(y \mid \tilde{\mathbf{a}}(\tilde{y}))$ in analogy to $\mathbf{a}$ and $f_Y(y \mid \mathbf{a})$, respectively. For instance, $\mathbf{a} = \{y_0, u(y_0)\}$ in ISO/FDIS 11929[2] becomes $\tilde{\mathbf{a}}(\tilde{y}) = \{\tilde{y}, \tilde{u}(\tilde{y})\}$. For more details, see the basic example of a counting measurement in Appendix 1. Not only x_1 but also the whole $\mathbf{x}$ can be influenced by $\tilde{y}$ as in the case of spectrum unfolding also shown in Appendix 1.

It is often sufficient to use as an approximation of the function $\tilde{\mathbf{a}}(\tilde{y})$ an interpolation of the sets $\mathbf{a}_j$ belonging to the results y_j from some previous measurements of the same kind carried out on samples with differing activities, but in other respects as far as possible under similar conditions. One of these measurements can be a background or blank measurement with $y_j = 0$. The measurement currently carried out can be taken as another one with $y_j = y_0$. The values y_j serve as the interpolation abscissas of the variable $\tilde{y}$.

INTEGRALS REPRESENTING THE BEST ESTIMATE, UNCERTAINTY AND CHARACTERISTIC LIMITS

In many cases, the functional values of the estimator distributions cannot explicitly be calculated for particular argument values y, since analytical formulas or algorithms required for solving the complicated integrals in equation (3) are often missing. Only argument values can be obtained by MC sampling from a preceding probability analysis according to references (14,15,21). This is the reason why the following integrals of the distributions then need to be calculated by MC and not more easily by the Simpson or similar numeric integration methods[27].

The best estimate of the measurand, the standard uncertainty associated with this best estimate, and the lower and upper limits of the coverage interval are defined in the following by means of moments and quantiles of the distributions $f_Y(y \mid \mathbf{a})$ and $f_Y(y \mid \mathbf{a},\ y \geq 0)$. The definitions of the decision threshold and the detection limit are based similarly on the distribution $f_Y(y \mid \tilde{\mathbf{a}}(\tilde{y}))$ with different assumed true measurand values $\tilde{y}$. The *p-quantile* of a distribution $f_Z(\zeta)$ is the upper integral limit q in the equation $\int_{-\infty}^{q} f_Z(\zeta)\mathrm{d}\zeta = F_Z(q) = \Pr(Z \leq q) = p$ with the given probability p. The particular probabilities α and β of the *errors of the first and second kind,* respectively, and the *coverage probability* $(1 - \gamma)$ used in the following have to be specified. For I_0, see equation (4). For illustrations of the distributions and the characteristic limits, see Figures 1 and 2.

The *best estimate* $\widehat{y}$ of the measurand Y is the expectation of the distribution $f_Y(y \mid \mathbf{a},\ y \geq 0)$:

$$\widehat{y} = \mathrm{E}(Y \mid \mathbf{a}, y \geq 0) = \frac{I_1}{I_0}; \qquad I_1 = \int_0^\infty y f_Y(y \mid \mathbf{a})\mathrm{d}y. \tag{6}$$

The *standard uncertainty* $u(\widehat{y})$ of the measurand associated with $\widehat{y}$ is the standard deviation of the distribution $f_Y(y \mid \mathbf{a},\ y \geq 0)$. It reads

$$u(\widehat{y}) = \sqrt{\mathrm{Var}(Y \mid \mathbf{a}, y \geq 0)} = \sqrt{\frac{I_2}{I_0} - \widehat{y}^2}; \qquad I_2 = \int_0^\infty y^2 f_Y(y \mid \mathbf{a})\mathrm{d}y. \tag{7}$$

The *lower limit* $y^{\triangleleft}$ *of the coverage interval* is the

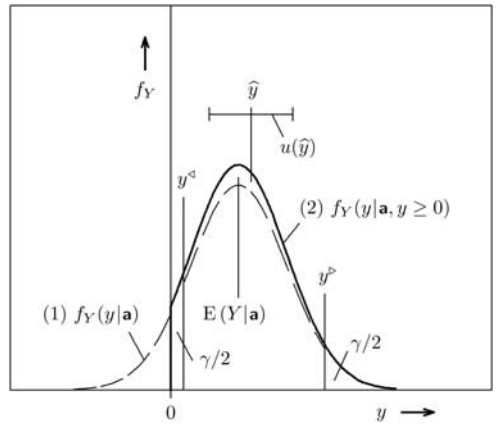

Figure 1. Illustration of the best estimate $\widehat{y}$ (expectation of distribution (2)) of a non-negative measurand Y with the associated standard uncertainty $u(\widehat{y})$ (standard deviation), and the limits $y^{\triangleleft}$ and $y^{\triangleright}$ of the coverage interval that covers the true measurand value with the probability $1 - \gamma$. The dashed line represents the distribution (1) of the possible true measurand values y, based on the available information $\mathbf{a}$ (from the measurement evaluated according to GUM[1]). By adding the condition $y \geq 0$ to $\mathbf{a}$, the distribution (1) is truncated at $y = 0$ and renormalised to form the boldface distribution (2). This leads to $y^{\triangleleft} \geq 0$.

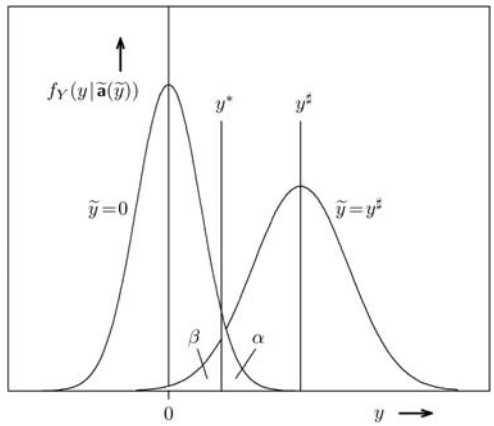

Figure 2. Illustration of the decision threshold y^* and the detection limit $y^\sharp$ of a non-negative measurand Y. The figure shows the distributions $f_Y(y\,|\,\tilde{\mathbf{a}}(\tilde{y}))$ of possible measurand estimates y from a measurement if the true values (expectations and parameter values) $\tilde{y}=0$ and $\tilde{y}=y^\sharp$ of Y are assumed. If $y_0 > y^*$ for a particular primary estimate y_0 from a measurement, then it is decided that the radiation effect quantified by Y is recognised as present. The areas α and β below the distributions on the right-hand and left-hand side of the abscissa y^* are the probabilities of the errors of the first and second kind, respectively. The area α 'covers' a piece of the line for $\tilde{y}=y^\sharp$.

$(\gamma/2)$-quantile of the distribution $f_Y(y\,|\,\mathbf{a}, y\geq 0)$:

$$F_Y(y^\triangleleft\,|\,\mathbf{a},\, y\geq 0)=\frac{\gamma}{2}=\frac{I_3}{I_0};$$
$$I_3=\int_0^{y^\triangleleft} f_Y(y\,|\,\mathbf{a})\mathrm{d}y=F_Y(y^\triangleleft\,|\,\mathbf{a})-F_Y(0\,|\,\mathbf{a}). \tag{8}$$

The *upper limit* $y^\triangleright$ *of the coverage interval* is the $(1-\gamma/2)$-quantile of the distribution $f_Y(y\,|\,\mathbf{a},\, y\geq 0)$:

$$1-F_Y(y^\triangleright\,|\,\mathbf{a}, y\geq 0)=\frac{\gamma}{2}=\frac{I_4}{I_0};$$
$$I_4=\int_{y^\triangleright}^{\infty} f_Y(y\,|\,\mathbf{a})\mathrm{d}y=1-F_Y(y^\triangleright\,|\,\mathbf{a}). \tag{9}$$

Although the integrals of equations (4) and (6)–(9) refer to the distribution $f_Y(y\,|\,\mathbf{a},\, y\geq 0)$, only the function $f_Y(y\,|\,\mathbf{a})$ is needed.

The measurement uncertainty $u(y)$ associated with an arbitrary estimate y is in general given by $u(y)=\sqrt{\mathrm{E}((Y-y)^2)}$[14,15] where $E((Y-y)^2)$ is the non-central second-order moment with respect to y. Accordingly, $u(y)$ assumes with $y=\mathrm{E}(Y)$ its minimum value, the standard deviation $\sqrt{\mathrm{Var}(Y)}$ of Y, also called the *standard uncertainty* [23 (2.30)]. The expectation $\mathrm{E}(Y)$ is therefore taken as the 'best' estimate $\hat{y}$ of the measurand Y and, together with the associated standard uncertainty $u(\hat{y})$, as the *measurement result* [23 (2.9)].

The *coverage interval* [21 (3.12), 23 (2.36)] between the limits according to equations (8) and (9) contains the true value of the measurand with the specified *coverage probability* $(1-\gamma)$ [21 (3.13), 23 (2.37)]. It is identical with the (*Bayesian*) *confidence interval* of the references cited, but it is merely analogous to the *confidence interval* in CS. The limits of the coverage interval are sometimes also called the *credible limits*. The coverage interval as defined above is *probabilistically symmetric* [21 (3.15)] as in common practice and ISO/FDIS 11929[2] for historical and practical demands. Other stipulations are possible. If, for instance, $\hat{y}$ in seldom cases happens not to be contained in the coverage interval, then the median m, defined by $F_Y(m\,|\,\mathbf{a},\ y\geq 0)=1/2$ and, thus, always contained in the coverage interval, may be taken as a reasonable estimate of the measurand, but with a larger associated uncertainty $u(m)=\sqrt{\mathrm{E}((Y-m)^2)}>u(\hat{y})$. If the true value 0 of the measurand is required to be always contained in the coverage interval, then $y^\triangleleft=0$ and $y^\triangleright$ defined by $F_Y(y^\triangleright\ |\ \mathbf{a}, y\geq 0)=1-\gamma$ could be stipulated. However the coverage interval is stipulated, it does not enlarge the knowledge of the measurand since all the information available and taken into account is already represented by the distribution $f_Y(y\,|\,\mathbf{a},\, y\geq 0)$.

The *decision threshold* y^* is the $(1-\alpha)$-quantile of the distribution $f_Y(y\,|\,\tilde{\mathbf{a}}(\tilde{y}=0))$ for the assumed true value $\tilde{y}=0$ of the measurand:

$$1-F_Y(y^*\,|\,\tilde{\mathbf{a}}(\tilde{y}=0))$$
$$=I_5=\int_{y^*}^{\infty} f_Y(y\,|\,\tilde{\mathbf{a}}(\tilde{y}=0))\mathrm{d}y=\alpha. \tag{10}$$

The *detection limit* $y^\sharp$ is the assumed true value of the measurand if the decision threshold y^* is the β-quantile of the distribution $f_Y(y\ |\ \tilde{\mathbf{a}}(\tilde{y}=y^\sharp))$:

$$F_Y(y^*\,|\,\tilde{\mathbf{a}}(\tilde{y}=y^\sharp))$$
$$=I_6=\int_{-\infty}^{y^*} f_Y(y\,|\,\tilde{\mathbf{a}}(\tilde{y}=y^\sharp))\mathrm{d}y=\beta. \tag{11}$$

Equations (10) and (11) also read $1-P(0)=\alpha$ and $P(y^\sharp)=\beta$, respectively, with the function $P(\tilde{y})=F_Y(y^*\,|\,\tilde{\mathbf{a}}(\tilde{y}))=\int_{-\infty}^{y} f_Y(y\,|\,\tilde{\mathbf{a}}(\tilde{y}))\mathrm{d}y$. Possibly, equation (11) has no unique solution $y^\sharp$ or even no solution at all. Therefore, a more general mathematical definition of the detection limit is needed and could read as follows: the detection limit is the

minimum true value $y^\sharp$ for which the *suitability condition* $P(\widetilde{y}) \leq \beta$ is met for all $\widetilde{y} \geq y^\sharp$. If there is no solution, then $y^\sharp = \infty$ is set. $P(\widetilde{y})$ is assumed to be a continuous function.

The decision threshold y^* and the detection limit $y^\sharp$ should be known before a measurement is carried out on a sample to be tested for ionising radiation. If $y_0 > y^*$ for a primary estimate y_0 from a measurement, then it is decided that the radiation effect in question, quantified by the measurand Y, is recognised as present. This decision is wrong and is called an *error of the first kind* if the radiation effect is actually absent. This case is assumed by choosing the true measurand value $\widetilde{y} = 0$. Its probability α is expressed by equation (10) (see Figure 2). ISO/FDIS 11929[2] requires to determine the best estimate $\widehat{y}$, the associated standard uncertainty $u(\widehat{y})$, and the limits $y^\triangleleft$ and $y^\triangleright$ of the coverage interval only if $y_0 > y^*$.

Notice that the condition $y \geq 0$ is not involved in the definitions of the decision threshold y^* and the detection limit $y^\sharp$ according to equations (10) and (11), respectively, since y_0, which has to be compared with y^*, is taken as obtained directly from the measurement data evaluation according to GUM[1] where the condition is ignored. Therefore, y^* must also be defined without the condition. This applies also to $y^\sharp$ since it depends on y^*. See also paragraph (a) of the concluding section.

If $y^\sharp \leq y_\mathrm{r}$ with a guideline value y_r specified for scientific, legal or other demands, then it is decided that the measurement procedure is suitable for the intended measurement purpose. Assume a present radiation effect by any true measurand value $\widetilde{y} > 0$. Then the decision that the radiation effect is recognised as absent—because of $y_0 \leq y^*$— is wrong and called an *error of the second kind*. The function $P(\widetilde{y})$ defined below equation (11) is the probability of this wrong decision. It must meet the suitability condition $P(\widetilde{y}) \leq \beta$ for all $\widetilde{y} \geq y^\sharp$ (see Figure 2) if $y_0 > y^*$, i.e. in the case of the decision that the radiation effect is recognised as present. For $\widetilde{y} = y_\mathrm{r} \geq y^\sharp$, in particular,

$$I_7 = P(y_\mathrm{r}) = \int_{-\infty}^{y^*} f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y} = y_\mathrm{r}))\mathrm{d}y \leq \beta. \qquad (12)$$

Vice versa, if $P(\widetilde{y}) \leq \beta$ for all $\widetilde{y} \geq y_\mathrm{r}$, then $y^\sharp \leq y_\mathrm{r}$ since $y^\sharp$ is a minimum value with respect to the suitability condition. Hence, it follows that the detection limit $y^\sharp$ is not needed if only the suitability decision has to be made with a given y_r. If $P(\widetilde{y})$ is known to decrease monotonously, then the condition $P(y_\mathrm{r}) \leq \beta$ is easier to test than $y^\sharp \leq y_\mathrm{r}$ and is sufficient for the suitability decision.

Since $\widetilde{y}$ is an assumed true measurand value, the expectation of the distribution $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ should meet the condition

$$\mathrm{E}(Y \mid \widetilde{\mathbf{a}}(\widetilde{y})) = \widetilde{y} \qquad (13)$$

in analogy to equation (6). Moreover, $\mathrm{Var}(Y \mid \widetilde{\mathbf{a}}(\widetilde{y})) = \widetilde{u}^2(\widetilde{y})$ is the squared uncertainty function $\widetilde{u}(\widetilde{y})$ used in ISO/FDIS 11929[2] and similar to equation (7).

The definitions given in equations (6)–(11) are in accordance with ISO/FDIS 11929[2]. But in this document, Gaussian distributions are used for $f_Y(y \mid \mathbf{a})$ and $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$. These distributions follow from the PME (see the next section) if, as an approximation and according to GUM[1], only their expectations y_0 and $\widetilde{y}$ and standard deviations $u(y_0)$ and $\widetilde{u}(\widetilde{y})$, respectively, are taken into account as constraints and form the information sets $\mathbf{a} = \{y_0, u(y_0)\}$ and $\widetilde{\mathbf{a}}(\widetilde{y}) = \{\widetilde{y}, \widetilde{u}(\widetilde{y})\}$.

ESTABLISHING DISTRIBUTIONS

PME and Bayes and expansion theorems

For the application of the MC method, the input distribution $f_\mathbf{X}(\boldsymbol{\xi} \mid \mathbf{a})$ according to equation (3) has to be formed. This task is described in detail in the GUM supplement[21] and in the Bayesian theory of measurement uncertainty[14,15]. A short introduction thus will be sufficient here.

The distribution $f = f_\mathbf{Z}(\boldsymbol{\zeta} \mid \mathbf{a})$ of any random variables $\mathbf{Z}$ can in general be obtained from actually available information $\mathbf{a}$ by using the PME[10–15] or other means such as the *Bayes theorem* or the *expansion theorem* of the probability theory. The PME is a fundamental, first principle in BS and in the uncertainty theory. It plays a part similar to other famous variational principles in physics like that of extremal action. Its importance should therefore not be underestimated. The Bayes and expansion theorems can be applied to include known frequency or parameter distributions, respectively. If possible and suitable, the mentioned methods can be applied alternatively, in combination, or in succession. If two of them are alternatively applicable in a particular case, then their results f must be identical provided that the same information is in analogy and correctly taken into account.

The PME consists in choosing as $f = f_\mathbf{Z}(\boldsymbol{\zeta} \mid \mathbf{a})$ the most likely distribution by taking into account relevant information available at present as so-called *constraints* and maximising the entropy

$$S = -\int_\mathbf{R} f \ln \frac{f}{f_0} \,\mathrm{d}\boldsymbol{\zeta} = \max \qquad (14)$$

by applying a variational method. $\mathbf{R}$ is the region of all possible values $\boldsymbol{\zeta}$ of $\mathbf{Z}$ and $f_0 = f_{0,\mathbf{Z}}(\boldsymbol{\zeta})$ is the *prior*, the distribution of $\mathbf{Z}$ based on the information

already known and included before the new information **a**, represented by **R** and the constraints, became available. If nothing was known before, then the prior is uniform. Only this case is assumed by the PME application of the GUM supplement [21 (6.3.2)]. The distribution f vanishes outside **R**. It is stressed once more that this solution of the PME depends essentially on the—nearly always incomplete—information available and taken into account. There is thus no 'true' distribution in BS.

If only the region **R** is known, then f is a uniform distribution in **R**. If constraints $\mathrm{E}(g_i(\mathbf{Z})) = d_i$ have to be met with given functions $g_i(\mathbf{Z})$ and data d_i, then the maximisation can be carried out by the Lagrange method (see any textbook on variational methods, e.g. reference[28]) and results for $\boldsymbol{\zeta} \in \mathbf{R}$ in

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{a}) = C f_{0,\mathbf{Z}}(\boldsymbol{\zeta}) \exp\left(-\sum_i \mu_i g_i(\boldsymbol{\zeta})\right). \quad (15)$$

The normalisation constant C and the coefficients μ_i, also called the *Lagrange multipliers*, have to be determined from the normalisation condition of a distribution and the constraints.

If there are no constraints, then $f = Cf_0$ inside **R** and $f = 0$ outside **R**. This leads to equation (4) with $\mathbf{Z} = Y$; $\boldsymbol{\zeta} = y$; $\mathbf{R} = \{y \mid y \geq 0\}$; $f = f_Y(y \mid \mathbf{a},\ y \geq 0)$ and the prior $f_0 = f_Y(y \mid \mathbf{a})$, which is taken as already known and updated by equation (4) for the condition $y \geq 0$.

If, in particular, $\mathbf{Z} = \mathbf{X}$ and only the expectation $\mathrm{E}\mathbf{X} = \mathbf{x}$ and the non-singular uncertainty (covariance) matrix $\mathbf{U}_\mathbf{x}$ associated with **x** are known and taken into account such that $\mathbf{a} = \{\mathbf{x}, \mathbf{U}_\mathbf{x}\}$ and, moreover, the prior is uniform and **R** is the whole ν-dimensional **X**-space, then a Gaussian distribution f is obtained:

$$f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{x}, \mathbf{U}_\mathbf{x}) = \frac{\exp\left(-\frac{1}{2}(\boldsymbol{\xi} - \mathbf{x})^\top \mathbf{U}_\mathbf{x}^{-1}(\boldsymbol{\xi} - \mathbf{x})\right)}{\sqrt{(2\pi)^\nu \det \mathbf{U}_\mathbf{x}}}. \quad (16)$$

In this case, $f_Y(y \mid \mathbf{a})$ according to equation (3) is also a Gaussian distribution if $G(\mathbf{X})$ is a linear function.

The also important Bayes theorem in the form

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v}) f_{\mathbf{V}}(\mathbf{v}) = f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta}) f_{1,\mathbf{Z}}(\boldsymbol{\zeta}) \quad (17)$$

can be applied if the *likelihood*, a (frequency) distribution $f\mathbf{V}(\mathbf{v} \mid \boldsymbol{\zeta})$ of random variables **V** with values **v**, being parts of the information **a**, and the prior $f_1 = f_{1,\mathbf{Z}}(\boldsymbol{\zeta})$ are available from previous measurements, experience or reasonable assumptions. But relative frequencies of such a distribution mean probability in the CS sense, whereas the BS sense is needed in the Bayes theorem. Both senses must therefore be identified. This will be, however, not of great importance in practice because of the asymptotic equivalence of BS and CS. Since **v** is fixed, $f_\mathbf{V}(\mathbf{v})$ is a constant $1/C$. The subscript 1 in equation (17) only indicates that the prior f_1 differs from f and f_0 in the PME according to equations (14) and (15). Hence, follows

$$f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{v}) = C f_{\mathbf{V}}(\mathbf{v} \mid \boldsymbol{\zeta}) f_{1,\mathbf{Z}}(\boldsymbol{\zeta}). \quad (18)$$

This distribution can be taken as the final f if no further information such as **R** or constraints has to be included. Otherwise, it must be used as the prior f_0 of the PME.

An example of the likelihood is the Poisson frequency distribution $f_\mathbf{V}(\mathbf{v} \mid \boldsymbol{\zeta}) = f_N(n \mid \varrho)$ with the counting variable $\mathbf{V} = N$, its recorded value $\mathbf{v} = n$ and the expectation $\mathrm{E}(N) = \varrho t$. Here, $\boldsymbol{\zeta} = \varrho$ is the possible true value of the count rate $\mathbf{Z} = R$ to be determined and t is the duration of the measurement. The distribution $f_\mathbf{Z}(\boldsymbol{\zeta} \mid \mathbf{v}) = f_R(\varrho \mid n)$ becomes a gamma distribution if, for instance, the prior $f_{1,\mathbf{Z}}(\boldsymbol{\zeta}) = f_R(\varrho) = H(\varrho)$ is applied since $\varrho \geq 0$ (see also equation (4) and the first example in Appendix 1). Although $f_N(n \mid \varrho) = \Pr(N = n \mid R = \varrho)$ is not a probability density but a probability function since N is a discrete random variable, this does not matter in the Bayes theorem.

The expansion theorem, also called the *theorem of total probability*, reads

$$f_{2,\mathbf{Z}}(\boldsymbol{\zeta}) = \int f_{\mathbf{Z}}(\boldsymbol{\zeta} \mid \mathbf{w}) f_{\mathbf{W}}(\mathbf{w}) \mathrm{d}\mathbf{w}. \quad (19)$$

Its output distribution f_2 can be taken as the final f if the distributions of the integrand, which depend on values **w** of parameters **W**, are given, for instance, as results from the PME or as priors. $f_\mathbf{W}(\mathbf{w})$ can also express a distribution of weights assigned to the values **w**. The expansion theorem can be obtained in a way similar to equations (1) and (2).

Additional remarks

There are cases where an update has to be made for new, additional information of the measurand. This can be done in several ways depending on the kind of information:

(a) The model equations can be refined by introducing new input quantities X_i. e.g. influence quantities, if the information refers to these quantities.
(b) The PME can be applied if the new information refers to the region **R** of the possible true values of the measurand or to the

constraints. Then, the old distribution f has to be used as the prior f_0.

(c) A distribution of a quantity Z, e.g. a prior, which will be more reasonable than a first assumed one such as a uniform prior over an interval, can be established by *Bayesian updating*[12] if a pool of comparable data z_k from previous, similar measurements is available. The improved distribution is then obtained, for instance, by fitting a suitably assumed function to the data[29]. These data, ordered by magnitude and renumbered as $z^{(k)}$, can also be used like the MC samples $y^{(k)}$ in equation (20). A suitably assumed inverse distribution function fitted to the M points $(k/M,\ z^{(k)})$ can be advantageous to the MC sampling treated in the following section.

(d) If a new prior, possibly improved according to (c), of the measurand or of a parameter or a distribution of weights have to be taken into account, then either the product rule according to equation (1) or the Bayes or expansion theorems according to equations (18) and (19) can be applied.

If the ν input components X_i of $\mathbf{X}$ are known to be independent random variables or nothing is known about their mutual dependence, then $f_{\mathbf{X}}(\boldsymbol{\xi}\,|\,\mathbf{a}) = \prod_{i=1}^{\nu} f_{X_i}(\xi_i\,|\,\mathbf{a}_i)$ with $\mathbf{a} = \{\mathbf{a}_1, \ldots, \mathbf{a}_\nu\}$. In multi-channel spectrum unfolding, all the $f_{X_i}(\xi_i\,|\,\mathbf{a}_i)$ are gamma distributions of the count rates $X_i = R_i$ and $\xi_i = \varrho_i$ with $\mathbf{a}_i = n_i$ (see the example of spectrum unfolding in Appendix 1).

According to the *central limit theorem* of probability theory, $f_Y(y\,|\,\mathbf{a})$ becomes in most cases, but with some exceptions, at least when standardised by the substitution $Y' = (Y - \mathrm{E}(Y))/\sqrt{\mathrm{Var}(Y)}$, an approximation of a (standardised) Gaussian distribution even if $f_{\mathbf{X}}(\boldsymbol{\xi}\,|\,\mathbf{a})$ is non-Gaussian. But the expectations $\mathbf{x}$ and the uncertainty matrix $\mathbf{U}_\mathbf{x}$ of $\mathbf{X}$ must exist and none of the ν input quantities X_i should strongly dominate by uncertainty. There should be more than only some few dimensions ν, but ν need not necessarily be a large number. But if ν tends to infinity as in multi-channel spectrum unfolding, then the expectation and the variance of Y should remain finite. Moreover, the model function $G(\mathbf{X})$ must be sufficiently linear in a neighbourhood of $\mathbf{x}$ determined by the condition $(\boldsymbol{\xi} - \mathbf{x})^\top \mathbf{U}_\mathbf{x}^{-1} (\boldsymbol{\xi} - \mathbf{x}) <\approx \nu$. If all these conditions are (nearly) met and, accordingly, $f_Y(y\,|\,\mathbf{a})$ is (approximately) a Gaussian distribution, ISO/FDIS 11929 can be applied directly. Then, an MC calculation is not necessary. This is an important result especially for spectrum unfolding. There are other, similar limit theorems making possible analytical or, for instance, iterative numerical approaches to multi-dimensional problems competing with MC methods[30].

Nevertheless, one should be cautious. If $f_Y(y\,|\,\mathbf{a})$ can indeed be well approximated by a Gaussian distribution, this applies mainly to the bulk of the distribution, but not necessarily to the tails that play a prominent part in the integrals I_4 to I_7 since α, β, and γ are commonly specified as small numbers. The same applies to the integral I_3 if $\widehat{y} \gg u(\widehat{y})$. If simple approximate arithmetic expressions for the distribution tails are known, then the contributions of the tails to the mentioned integrals can possibly be better calculated analytically than by MC.

There are cases where the PME seems to have no solution[31]. Let, for instance, an estimate x (expectation) and the associated standard uncertainty $u(x)$ (standard deviation) be given for a measurand X known to be valued in some interval between a and $b > a$. If x is not contained in the interval or $u(x) > b - a$, then, indeed, there is no solution from the PME for the distribution $f = f_X(\xi\,|\,x, u(x), a, b)$ to be determined. What does this mean? It merely indicates that there is something wrong with the information. The information is contradictory or badly interpreted. This should give an incentive to carefully inspect the measurement and the data evaluation in order to find the reason for the inconsistency. The first question should be: How are x and $u(x)$ obtained from what information? Suppose, for instance, that x and $u(x)$ are determined from measurement data v_i according to GUM[1] as the arithmetic mean and the empirical standard deviation (type A evaluation of measurement uncertainty [23 (2.28)]), respectively. The interval information a and b has not yet been used. Thus, x and $u(x)$ do *not* belong to the distribution f but to a distribution $f_0 = f_X(\xi\,|\,x, u(x))$! GUM does not provide this distribution but f_0 can be reconstructed by the PME with a uniform prior and turns out to be the Gaussian distribution $f_0 = \exp(-(\xi - x)^2/(2u^2(x)))/\sqrt{2\pi u^2(x)}$. This distribution must now be subsequently updated for the additional interval information to form the final distribution f. This can again be done by the PME but f_0 must now act as the prior since it represents the knowledge already taken into account. Then, equation (14) has to be solved for f with $\mathbf{Z} = X; \boldsymbol{\zeta} = \xi$ and $\mathbf{R} = \{\xi\,|\,a \le \xi \le b\}$ and with the normalisation condition only. Equation (15), where the sum now vanishes, yields $f = Cf_0$ for $\xi \in \mathbf{R}$ and $f = 0$ elsewhere. Thus, f_0 is truncated at a and b and renormalised to form f. There is always a solution f. Naturally with f, the 'best' estimate now turns out to be $\widehat{x} = \mathrm{E}(X) \neq x$ with $a \le \widehat{x} \le b$ and $u(\widehat{x}) = \sqrt{\mathrm{Var}(X)} \le \min(u(x), b - a)$. All possible coverage intervals are contained in the interval between a and b. The prior f_0 introduced in the PME here reasonably eliminates the difficulty. The example treated here is similar to subsequently taking into account the condition $y \ge 0$ for a non-negative

measurand Y as is shown below equation (15). In this case, $a = 0$ and $b = \infty$.

MC DATA SAMPLING

The point of view now changes from the fundamentals on the metrological level to the numerics on the MC level.

With the MC method, a very large number N of values $\mathbf{x}_k$, called the *samples*, are drawn from the distribution $f_{\mathbf{X}}(\mathbf{x} \mid \mathbf{a})$ and values $y_k = G(\mathbf{x}_k)$ are calculated ($k = 1, \ldots, N$). Although this MC data sampling is already comprehensively described in the GUM supplement[21], some additional, more general aspects are treated here, which could be important for the calculation of integrals in the present paper. These aspects concern uncertainty contributions induced by the MC method and the *importance sampling random walk*[32,33], which offers a possibility of reducing considerably the number N of samples needed.

In many cases, some or all components of $\mathbf{X}$ are independent of the other ones and each have a strictly increasing, continuous distribution function $F_{X_i}(\xi)$. Then, with a random number θ drawn by means of a random-number generator from a uniform distribution between 0 and 1, the θ-quantile x satisfying $F_{X_i}(x) = \theta$ is a sample of X_i. In the following, θ is called a *standard random number*. The sequence of all standard random numbers θ used during an MC run is called a *history*. A shortcoming of the general sampling method just described is that the inverted distribution function must be available, for instance, from a pre-computed table, in order to calculate the θ-quantiles rapidly enough. Other methods of generating samples, e.g. the acceptance–rejection method, are described in references[33,34] and elsewhere.

Distribution function

For the determination of the characteristic limits, an approximation $\widetilde{F}_Y(y \mid \mathbf{a})$ of the distribution function $F_Y(y \mid \mathbf{a})$ is useful and is prepared as follows. After the sampling, if necessary, the N values y_k are sorted by magnitude and renumbered by $y^{(k)}$ such that $y^{(k)} \le y^{(k+1)}$. Only these N values $y^{(k)}$ are stored as the results of the MC run and as the abscissas of the distribution function. This way of storing the data is called the *sample-storing mode* in the following. After the MC run has been carried out, the corresponding ordinate values $\widetilde{F}_Y(y^{(k)} \mid \mathbf{a}) = k/N$ are then set and, in addition, $\widetilde{F}_Y(y \mid \mathbf{a}) = 0$ for $y < y^{(1)}$ and $\widetilde{F}_Y(y \mid \mathbf{a}) = 1$ for $y > y^{(N)}$. For $y^{(k)} < y < y^{(k+1)}$, a linear interpolation is applied. An interpolated functional value is

$$\widetilde{F}_Y(y \mid \mathbf{a}) = \frac{1}{N}\left(k + \frac{y - y^{(k)}}{y^{(k+1)} - y^{(k)}}\right) \qquad (y^{(k)} < y < y^{(k+1)}) \tag{20}$$

In this way, the approximation $\widetilde{F}_Y(y \mid \mathbf{a})$ becomes a continuous, piecewise linear, and between $y^{(1)}$ and $y^{(N)}$ strictly increasing function. Obviously, the functional values need not be stored since they can easily be determined after the MC run if necessary.

During the MC run, several counters of interest, denoted by $N(\text{conditions} \mid \text{parameters})$, are incremented if y_k meets the conditions. For instance, $N(y_k \le \eta)$ means the number of samples $y_k \le \eta$. If suitably chosen abscissas η_j ($j = 1, \ldots, M \ll N$) with $\eta_j < \eta_{j+1}$ are introduced, then the M counters $n_j = N(y_k \le \eta_j)$ represent something like an accumulated 'multi-channel spectrum'. Then, $\widetilde{F}_Y(\eta_j \mid \mathbf{a}) = n_j/N$ can serve as an alternative approximation of the distribution function defined similar to that described above. The advantages of this *multi-channel mode* are that only the $M \ll N$ number pairs (η_j, n_j) need to be stored and sorting can be avoided, but larger MC-induced uncertainties must possibly be accepted as a shortcoming. Now, an interpolated functional value is

$$\widetilde{F}_Y(y \mid \mathbf{a}) = \frac{n_j \cdot (\eta_{j+1} - y) + n_{j+1} \cdot (y - \eta_j)}{N \cdot (\eta_{j+1} - \eta_j)} \qquad (\eta_j < y < \eta_{j+1}). \tag{21}$$

The multi-channel mode is especially suited to the determination of a quantile q by using a few appropriately chosen approximations η_j of q. The MC-induced uncertainties associated with n_j and q in this case can be obtained according to Appendix 4.

The sample-storing and multi-channel modes can be combined. If, for instance, $\widetilde{F}_Y(y \mid \mathbf{a})$ is needed only in a known, possibly small range $a < y < b$, then $\widetilde{F}_Y(a \mid \mathbf{a}) = N(y_k \le a)/N$ and $\widetilde{F}_Y(b \mid \mathbf{a}) = 1 - N(y_k \ge b)/N$ can be set and only the samples falling into this range have to be sorted by magnitude and treated as described above.

General integral determination

In the following, I strictly denotes an integral and J its estimate or approximation. An integral

$$I = \int_{\mathbf{R}} L(\mathbf{x}) \mathrm{d}\mathbf{x} \tag{22}$$

of any function $L(\mathbf{x})$ over a fixed region $\mathbf{R}$ can be calculated by the MC method in the following way.

Bounds a_i and b_i are first chosen for each of the ν components x_i of $\mathbf{x}$ such that $a_i \le x_i \le b_i$ for all samples $\mathbf{x} \in \mathbf{R}$. The bounds a_i and b_i should be as large and as small, respectively, as possible such that the ν-dimensional cuboid defined by the bounds surrounds the region $\mathbf{R}$ as closely as possible. $V = \prod_{i=1}^{\nu}(b_i - a_i)$ is the volume of the cuboid. If $\mathbf{R}$ is infinite, it must be previously suitably transformed to become a finite region. The substitution $x_i = v_i/(1 - v_i^2)$, for instance, transforms an arbitrary region $\mathbf{R}$ of $\mathbf{x}$ to a finite region of $\mathbf{v}$ since there is a v_i with $|\, v_i\,| < 1$ for every X_i. Another example is the substitution $x_i = -\ln(v_i)$. For every $x_i \ge 0$, there is a v_i with $0 < v_i \le 1$.

Then, ν standard random numbers θ_i are drawn, i.e. $0 \le \theta_i \le 1$ $(i = 1, \ldots, \nu)$, and the components $x_i = a_i + (b_i - a_i)\theta_i$ of a sample $\mathbf{x}_k$ are formed. This is repeated N times for $k = 1, \ldots, N$. Here, N is a very large number of samples $\mathbf{x}_k$ generated in this way. If $\mathbf{x}_k \in \mathbf{R}$, then $L(\mathbf{x}_k)$ is calculated. Otherwise, $L(\mathbf{x}_k) = 0$ is set. With the functional values $L(\mathbf{x}_k)$, the (arithmetic) mean $\overline{L}$ and the variance $s^2(\overline{L})$ of the mean are determined:

$$\begin{aligned} J = V\overline{L} &= \frac{V}{N}\sum_{k=1}^{N} L(\mathbf{x}_k) \\ &= V\cdot\left(\frac{1}{N}\sum_{k=1}^{N}(L(\mathbf{x}_k) - L_0) + L_0\right); \end{aligned} \tag{23}$$

$$\begin{aligned} u_{\mathrm{MC}}^2(J) = V^2 s^2(\overline{L}) &= \frac{V^2}{N(N-1)}\sum_{k=1}^{N}(L(\mathbf{x}_k) - \overline{L})^2 \\ &= \frac{V^2}{N-1}\left(\frac{1}{N}\sum_{k=1}^{N}(L(\mathbf{x}_k) - L_0)^2 - (\overline{L} - L_0)^2\right) \end{aligned} \tag{24}$$

$u_{\mathrm{MC}}(J)$ is the MC-induced standard uncertainty of the integral I associated with the estimate J. The sample number N must be chosen large enough so that $u_{\mathrm{MC}}(J)$ can be neglected when compared with other uncertainty components, or it must also be taken into account. The last expressions in equations (23) and (24) are better suited for numeric calculations. This *Kahan summation* reduces the influences of rounding errors. L_0 is an arbitrary, but best-possible approximation of $\overline{L}$. The denominator $N - 1$ in equation (24) applies in CS. In BS, it has to be replaced by $N - 3$[22]. But -1 or -3 can be neglected since N should be very large, typically 10^6. This shows the asymptotical equivalence of BS and CS in the present case.

If J is taken as a random variable, an estimator of I, then $\mathrm{E}(J) = I$ and

$$\mathrm{Var}(J) = \frac{1}{N}\left(V\int_{\mathbf{R}} L^2(\mathbf{x})\mathrm{d}\mathbf{x} - I^2\right). \tag{25}$$

$u_{\mathrm{MC}}^2(J)$ according to equation (24) is an estimate of $\mathrm{Var}(J)$. Equation (25) means $\mathrm{Var}(J) = \mathrm{const}/N$. But the MC procedure is only meaningful if the integral of $L^2(\mathbf{x})$ exists. Moreover, this integral should be as small as possible. Its existence and reduction can also be achieved by a skilful transformation such that the integrand becomes uniform as far as possible. In the case of $I = \int_0^1 \mathrm{d}x/\sqrt{x}$, for instance, the integral of $L^2(x) = 1/x$ does not exist. But the substitution $x = v^2$ leads to $I = 2\int_0^1 \mathrm{d}v$ and even to $\mathrm{Var}(J) = 0$.

Importance sampling random walk

In many cases, a relatively small connected subregion $\mathbf{S} \subset \mathbf{R}$ mainly contributes to the integral I according to equation (22) if $L(\mathbf{x})$ nearly vanishes outside $\mathbf{S}$. Then it could be more practical to choose the samples $\mathbf{x}_k$ in such a way that their number density asymptotically for $N \to \infty$ becomes proportional to an available or suitably chosen probability density $f(\mathbf{x})$. By first setting $L(\mathbf{x}) = g(\mathbf{x})f(\mathbf{x})$, this can be done as follows whereby $\mathbf{S}$ need not be specified exactly.

Beginning with an arbitrary sample $\mathbf{x}_1 \in \mathbf{S}$, a sample $\mathbf{x}'$ is drawn from a uniform distribution in a small neighbourhood of $\mathbf{x}_k$, for instance, in a cuboid centred at this sample. $\mathbf{x}'$ is accepted as a new sample $\mathbf{x}_{k+1}$ if $\mathbf{x}' \in \mathbf{R}$ and $v = f(\mathbf{x}')/f(\mathbf{x}_k) \ge 1$ or, if $v < 1$, another random number θ yields $\theta < v$. Otherwise, $\mathbf{x}'$ is rejected and $\mathbf{x}_k$ is retained as $\mathbf{x}_{k+1}$. Then,

$$J = \overline{g} = \frac{1}{N}\sum_{k=1}^{N} g(\mathbf{x}_k) \tag{26}$$

is an estimate of I. The procedure described is called the *importance sampling random walk*[32,33]. The random walk automatically stays preferably inside the subregion $\mathbf{S}$. This can reduce considerably the number of samples needed if otherwise many samples far outside $\mathbf{S}$ would have had to be generated but could not contribute much to the integral.

A formula for the standard uncertainty $u_{\mathrm{MC}}(J)$ can be derived by analogy from equation (23) to equation (24). With VL replaced by g and with $h(\mathbf{x}) = g^2(\mathbf{x})f(\mathbf{x})$ and $\overline{h}$ similar to equation (26),

$$u_{\mathrm{MC}}^2(J) = \frac{V\overline{h} - J^2}{N-1} \tag{27}$$

results. Obviously, $u^2_{\mathrm{MC}}(J) \approx c/N$. But the constant c could be rather large. This requires a correspondingly large N to obtain a sufficiently small $u_{\mathrm{MC}}(J)$. This is due to the restricted choice of $\mathbf{x}'$ in the neighbourhood of $\mathbf{x}_k$. The neighbourhoods at the steps may arbitrarily be formed, but preferably in such a way that nearly half of the samples $\mathbf{x}'$ are rejected. It may be sufficient at every step to vary only one or a few randomly or cyclically chosen components of $\mathbf{x}_k$ in order to obtain $\mathbf{x}'$.

The importance sampling can be adequate and advantageous for quantiles as can easily be seen in the following. Every quantile can be written as a fraction $Q = I(\mathbf{Q})/I(\mathbf{R}) \leq 1$ of two integrals I of the same integrand but different integration regions $\mathbf{R}$ and $\mathbf{Q} \subset \mathbf{R}$. Here, $\mathbf{R}$ is the region of all possible samples $\mathbf{x}_k$ and $\mathbf{Q}$ is the subregion of all the samples $\mathbf{x}_k$ with $y_k = G(\mathbf{x}_k)$ contributing to the quantile. Instead of drawing N samples $\mathbf{x}_k$ from $\mathbf{R}$, a considerably smaller number $N' < N$ of samples is drawn by importance sampling mainly from the essential subregion $\mathbf{S} \subset \mathbf{R}$ and used to determine $I(\mathbf{R})$ that acts as the normalisation integral. Those of the samples yielding values $y_k = G(\mathbf{x}_k)$ belonging to the quantile are used for $I(\mathbf{Q})$. This means that the quantile $Q = I(\mathbf{Q})/I(\mathbf{R})$ is approximated by $I(\mathbf{Q} \cap \mathbf{S})/I(\mathbf{S})$ since samples $\mathbf{x}_k$ outside $\mathbf{S}$ barely contribute to the integrals.

MC CALCULATION OF THE INTEGRALS

Obviously, there are three types of integrals. (A) I_0, I_1, I_2 and I_7 have fixed integral limits and can be directly calculated by MC with suitably sampled values of the integration variable. (B) In I_3, I_4 and I_5, one of the integral limits has to be determined. (C) I_6 also has fixed integral limits, but a parameter of the integrand has to be calculated and the MC-induced uncertainty of one of the integral limits has to be taken into account (also for I_7). Types B and C can also be numerically determined by MC but require additional considerations.

Preliminary approximations of $f_Y(y \mid \mathbf{a})$ and of the integrals can be obtained according to references[2,17–19] by using a Gaussian distribution (see the two last but one paragraphs of the preceding section dealing with establishing input distributions).

If the characteristic limits or preliminary approximations of them are available, then MC approximations of the integrals I_0 and I_3 to I_7 useful for a test are:

$$I_0 \approx \frac{N(y_k \geq 0 \mid \mathbf{a})}{N}; \tag{28}$$

$$\frac{I_3}{I_0} = \frac{\gamma}{2} \approx \frac{N(0 \leq y_k < y^{\triangleleft} \mid \mathbf{a})}{N(y_k \geq 0 \mid \mathbf{a})}; \tag{29}$$

$$\frac{I_4}{I_0} = \frac{\gamma}{2} \approx \frac{N(y_k < y^{\triangleright} \mid \mathbf{a})}{N(y_k \geq 0 \mid \mathbf{a})} \tag{30}$$

since samples with $y^{\triangleleft} \leq y_k \leq y^{\triangleright}$ belong to the coverage interval.

$$I_5 = \alpha \approx \frac{N(y_k < y^* \mid \widetilde{\mathbf{a}}(\widetilde{y} = 0))}{N} \tag{31}$$

since samples $y_k > y^*$ falsely let the radiation effect be recognised as present although the assumed true value of the measurand is $\widetilde{y} = 0$ (error of the first kind).

$$I_6 = \beta \approx \frac{N(y_k \leq y^* \mid \widetilde{\mathbf{a}}(\widetilde{y} = y^{\sharp}))}{N}; \tag{32}$$

$$I_7 \approx \frac{N(y_k \leq y^* \mid \widetilde{\mathbf{a}}(\widetilde{y} = y_{\mathrm{r}}))}{N} \leq \beta \tag{33}$$

since samples $y_k \leq y^*$ falsely let the radiation effect be recognised as absent, although the assumed true value of the measurand is $\widetilde{y} > 0$ (error of the second kind).

A simple, but possibly not always economic method of determining the characteristic limits consists of several MC runs repeatedly carried out with the *same*(!) history of standard random numbers but varied approximations of the characteristic limits until equations (29)–(32) are fulfilled sufficiently well. After each run, the equations are tested and the approximations are cautiously changed with respect to the test results by a dialogue with the computer program. The decision threshold y^* must already be available before the detection limit $y^{\sharp}$ can be determined. The calculations should finally be followed by the determination of the MC-induced uncertainties associated with the obtained results according to the next section and Appendix 4.

Sometimes it is essential to calculate MC approximations $J(\eta_0)$ and $J(\eta_1)$ of any quantity I with slightly different parameter values η_0 and η_1, respectively, by using the *same* history of standard random numbers either simultaneously during the same MC run or in successive runs. Many random-number generators offer this mode. Random deviations then nearly cancel out in the difference $J(\eta_1) - J(\eta_0)$[35]. *Distinctly* generated histories can be taken as independent and should be used if a correlation, for instance, between $J(\eta_0)$ and $J(\eta_1)$ has to be avoided (see Appendix 4).

Type-A integrals

Estimates $J_0 = N(y_k \geq 0 \mid \mathbf{a})/N$ and J_1 and J_2 of the type-A integrals I_0, I_1 and I_2, respectively, are

obtained with $\mu = 0$, 1, 2 by the (arithmetic) mean values:

$$J_\mu = \overline{y^\mu H} = \frac{1}{N}\sum_{k=1}^{N} y_k^\mu H(y_k). \tag{34}$$

Then,

$$\widehat{y} \approx \frac{J_1}{J_0}; \quad u^2(\widehat{y}) \approx \frac{J_2}{J_0} - \left(\frac{J_1}{J_0}\right)^2. \tag{35}$$

The type-A integrals should always be accumulated during the same MC run since $N(y_k \geq 0 \,|\, \mathbf{a})$ for I_0 and the sums for I_1 and I_2 can easily be updated when a new sample y_k is drawn. The samples y_k need not be sorted by magnitude. Within CS on the MC level, the expressions given in equation (35) for $\widehat{y}$ and $u^2(\widehat{y})$ are, at least asymptotically for $N \to \infty$, unbiased estimates of the expectation and the variance, respectively, of the distribution $f_Y(y \,|\, \mathbf{a}, y \geq 0)$. A possible bias is neglected since N is a very large number, typically 10^6 (see text below equation (24)). The uncertainty $u(\widehat{y})$ should not be confused with the MC-induced uncertainty $u_{\mathrm{MC}}(\widehat{y})$ that expresses how accurately $\widehat{y}$ is calculated by MC (see the next section and Appendix 4). The integral I_7 can be obtained in a similar manner to I_0. See also the following subsection.

Type-B integrals

The type-B integrals I_3 and I_4 have the same integrand parameters represented by $\mathbf{a}$ as the type-A integrals I_0, I_1 and I_2. All these integrals can therefore be determined from the data of the same MC run, whereas the integral I_5 and the type-A integral I_7 require their own MC run because $\widetilde{\mathbf{a}}(\widetilde{y})$ differs from $\mathbf{a}$. The type-B integrals should preferably be calculated after the MC run has been carried out. They can be written in the generalised form

$$I(\eta) = \int_c^\eta f\,(x)\mathrm{d}x = \varepsilon \tag{36}$$

where c and ε are given constants and η is to be calculated. $f(x)$ is a distribution and $I(\eta)$ is a monotonously increasing function. Let $J(\eta)$ be the approximation of $I(\eta)$ obtained from the MC run. To solve equation (36), first search for the maximum and minimum η values, denoted by η_0 and η_1, respectively, such that $\eta_0 < \eta_1$ and $J(\eta_0) \leq \varepsilon$ and $J(\eta_1) \geq \varepsilon$ and apply a linear interpolation. This yields

$$\eta = \eta_0 + \frac{(\varepsilon - J(\eta_0)) \cdot (\eta_1 - \eta_0)}{J(\eta_1) - J(\eta_0)} \tag{37}$$

A higher order interpolation need not be carried out if the number N of MC samples is sufficiently large. Equation (37) can be applied to both the sample-storing mode and the multi-channel mode. In the latter mode it could happen, although it is unlikely, that several adjacent channels have the same contents $J(\eta) = \varepsilon$. Then the mean η of these channels should be taken as the solution η. The estimates $J(\eta_0)$ and $J(\eta_1)$ of the integrals should be calculated by using the same history of standard random numbers (see above in the present section and also the next section and Appendix 4). Otherwise, the MC-induced uncertainty of the denominator in equation (37) would become too large[35]. Preliminary estimates for an iterative application of equation (37) may be determined with a reduced N if computing time has to be saved.

The distribution function approximation $\widetilde{F}_Y(y \,|\, \mathbf{a})$ is involved to form the function $J(\eta)$ as in the type-B integrals I_3 and I_4. If the solution η is known to be located in the interval between available values a and $b > a$, then only the samples in this interval need to be sorted by magnitude and the numbers $N(y_k < a \,|\, \mathbf{a})$ or $N(y_k > b \,|\, \mathbf{a})$ must be counted. This is sufficient to determine the distribution function approximation in the interval.

Type-C integrals

Type-C integrals like I_6 have the form

$$I(\eta) = \int_a^b f\,(x;\eta)\mathrm{d}x = \varepsilon \tag{38}$$

that has to be solved for the function parameter η. The integral limits a and b and the integral value ε are given constants. With approximate values η_0 and η_1 for η, an improved approximation η is obtained similar to equation (37) with

$$J(\eta_j) = \frac{N(a \leq x_k \leq b \,|\, \eta_j)}{N} \tag{39}$$

for $j = 0$, 1. The relation symbols $\leq$ or $<$ depend on whether or not a and b belong to the integration interval.

MC-INDUCED UNCERTAINTY

An integral I can be calculated by MC as accurately as required by choosing a sufficiently large sample number N. That is, the MC-induced uncertainty $u_{\mathrm{MC}}(J) \sim 1/\sqrt{N}$ associated with an MC estimate J of I can be made arbitrarily small. But for every additional significant leading decimal digit of J, the number N and, thus, the computing time must be multiplied by 100. For computing economy, N

should therefore be chosen as small as reasonable. But how many samples are needed? And what about the MC-induced uncertainty $u_{\mathrm{MC}}(q)$ associated with a quantile estimate $q = J/J_0$ as a fraction of integral estimates J and J_0? Here, the correlation beween J and J_0 must also be taken into account when these estimates are calculated, again with the same history of standard random numbers. Such questions are analysed in Appendix 4. It is assumed that in most cases in practice, an accuracy of two or three significant leading digits will suffice for the characteristic limits. This means that an associated MC-induced relative uncertainty <0.01 (1%) is assumed to be required. To satisfy such a requirement, only upper bounds of the MC-induced uncertainties as small as possible need to be determined.

An easy way to assess MC-induced uncertainties consists in independently repeating an MC run ν times with different histories and looking for how many digits of any particular result z in question do not change. More accurately, the MC-induced uncertainty associated with z as one of the individual outcomes z_k of the ν runs is

$$u_{\mathrm{MC}}(z) = \sqrt{\frac{1}{\nu - 1}\sum_{k=1}^{\nu}(z_k - \overline{z})^2} \tag{40}$$

where $\overline{z}$ is the arithmetic mean of the z_k. If $\overline{z}$ is taken as the final result z, then the right-hand side of equation (40) must be divided by $\sqrt{\nu}$. A deeper insight into the matter can be obtained by the considerations in Appendix 4. An assessment of MC-induced uncertainties in advance could also be advantageous for MC programs under development.

CONCLUSIONS

The characteristic limits, estimates and associated uncertainties studied in the present paper are needed for the recognition, detection and quantification of ionising radiation and allow decisions to be made for radiation protection purposes. They are quite generally defined on BS as close as possible and reasonable to traditional, common practice and are calculated by using MC methods. This enables them to be applied even to complex and critical cases in radiation measurement. Moreover, the MC approach to the characteristic limits makes possible to go a step beyond the present state of standardisation laid down in ISO/FDIS 11929[2] since distributions rather than uncertainties can be propagated. It is thus more comprehensive and promising.

ISO/FDIS 11929[2] mainly uses Gaussian probability distributions. More general distributions representing all available, relevant knowledge of the radiation measurand in question can be obtained, e.g. by the PME, but require the application of MC. Sometimes, the distributions can be approximated by Gaussian ones if there is a parameter τ, for instance, the measurement duration, which can be made sufficiently large to improve the approximation. The convergence to the Gaussian distributions can in general be rather slow, only proportional to $1/\sqrt{\tau}$. There are remarkable differences in Appendix 3 between the results of the Gaussian and the MC approaches. This comes first from the intentional choice of the example such that the differences become significant and obvious. Nevertheless, this also shows that MC application can be necessary and advantageous in practice.

The question of whether or not the definitions of the characteristic limits are the best possible or most reasonable ones was not studied but should be discussed in the future to achieve common agreement. Some other definitions have already been considered. Two examples are:

(a) If $y_0 > y^*$, then it is decided that the radiation effect in question is recognised as present. Instead, the condition $\widehat{y} > y^{**}$ is proposed where y^{**} is defined similar to the decision threshold y^* according to equation (10) but with the distribution $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y} = 0))$ replaced by $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y} = 0), y \geq 0)$. Such a definition could be possible but is it an improvement? Since $y_0 \leq \widehat{y}$ and also $y^* \leq y^{**}$, this question cannot easily be answered. Moreover, the proposal requires more computing effort.

(b) If $y^\sharp \leq y_{\mathrm{r}}$, then it is decided that the measurement procedure is suitable. But the detection limit $y^\sharp$ needs much iterative MC computation. As shown in the text below equation (12), there is an equivalent condition $P(y_{\mathrm{r}}) \leq \beta$, which can be more easily tested since only a simple type-A integral has to be calculated by MC. The detection limit is not needed in this case.

Finally, because of often arising misunderstandings, it must be stressed once more, that every distribution used in the present work has to be interpreted in the Bayesian sense as representing just the information taken into account of a quantity in question. This also applies by a new interpretation to a frequency distribution involved in equations (17) and (18), e.g. the Poisson distribution. If the amount of information changes, then the distribution and all the results obtained from this distribution also change, including the characteristic limits. Naturally, additional information can, for instance, reduce the coverage interval. Accordingly, the matter of characteristic limits is not a matter of right or wrong but a matter of knowledge, approximation, reasonableness and expenditure as often in physics.

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REFERENCES

1. International Organization for Standardization. *Uncertainty of Measurement—Part 3: Guide to the Expression of Uncertainty in Measurement (GUM).* ISO/IEC Guide 98–3 (Geneva: ISO) (2008).
2. International Organization for Standardization. *Determination of characteristic limits (decision threshold, detection limit, and limits of the confidence interval) for measurements of ionizing radiation—fundamentals and applications.* ISO/FDIS 11929 (Geneva: ISO) (2008).
3. Berger, J. O. *Statistical decision theory and Bayesian analysis* (New York: Springer) (1985).
4. Bernardo, J. M. and Smith, A. F. M. *Bayesian theory* (Chichester: Wiley) (1994).
5. Bernardo, J. M. *Bayesian statistics.* In: Probability and Statistics. Encyclopedia of Life Support Systems (EOLSS). Viertl, R., Ed. (Oxford: UNESCO) (2003).
6. Gelman, A., Carlin, J. B., Stern, H. and Rubin, D. B. *Bayesian Data Analysis*, second edn. (London: Chapman) (2003).
7. Gregory, P. C. *Bayesian logical data analysis for the physical sciences* (Cambridge: Cambridge University Press) (2005).
8. Lee, P. M. *Bayesian statistics: an introduction* (New York: Oxford University Press) (1989).
9. Robert, C. P. *The Bayesian Choice*, second edn. (New York: Springer) (2001).
10. Rosenkrantz, R. D., Ed. *E.T. Jaynes: papers on probability, statistics and statistical physics* (Dordrecht: Kluwer Academic Publishers) (1989).
11. Jaynes, E. T. *Probability theory—The Logic of Science.* Bretthorst, G. L., Ed., (Cambridge: Cambridge University Press) (2003).
12. Sivia, D. S. *Data analysis: A Bayesian Tutorial*, second edn. Sivia, D. S. and Skilling, J., Eds. (New York: Oxford Press) (2006).
13. *Principle of maximum entropy.* http://en.wikipedia.org/wiki/Maximum_entropy. Last accessed on June 13 2009.
14. Weise, K. and Wöger, W. *A Bayesian theory of measurement uncertainty.* Meas. Sci. Technol. **4**, 1–11 (1993). Eine Bayessche Theorie der Messunsicherheit. PTB Report N–11 (Braunschweig: Physikalisch-Technische Bundesanstalt) (1992).
15. Weise, K. and Wöger, W. *Messunsicherheit und Messdatenauswertung (Measurement uncertainty and measurement data evaluation)* (Weinheim: Wiley-VCH) (1999) (in German).
16. Kacker, R. N. and Jones, A. T. *On use of Bayesian statistics to make the guide to the expression of uncertainty in measurement consistent.* Metrologia **40**, 235–248 (2003).
17. Weise, K. *Bayesian-statistical decision threshold, detection limit and confidence interval in nuclear radiation measurement.* Kerntechnik **63**, 214–224 (1998).
18. Weise, K., Hübel, K., Michel, R., Rose, E., Schläger, M., Schrammel, D. and Täschner, M. *Determination of the detection limit and decision threshold for ionizing-radiation measurements: fundamentals and particular applications—proposal for a standard.* Report FS-05-129-AKSIGMA, Fachverband für Strahlenschutz (Cologne: TÜV-Verlag) (2005).
19. Weise, K., Hübel, K., Rose, E., Schläger, M., Schrammel, D., Täschner, M. and Michel, R. *Bayesian decision threshold, detection limit and confidence limits in ionising-radiation measurement.* Radiat. Prot. Dosimetry **121**, 52–63 (2006).
20. International Organization for Standardization. *Determination of the detection limit and decision threshold for ionizing radiation measurements—Part 7: Fundamentals and general applications.* ISO 11929-7 (Geneva: ISO) (2005).
21. International Organization for Standardization. *Uncertainty of Measurement – Part 3: Guide to the Expression of Uncertainty in Measurement (GUM)—Supplement 1: Propagation of Distributions using a Monte Carlo Method.* ISO/IEC Guide 98-3/Suppl.1 (Geneva: ISO) (2008) and JCGM 101:2008. www.bipm.org/utils/common/documents/jcgm/JCGM_101_2008_E.pdf. Last accessed on June 13 2009.
22. Lira, I. and Wöger, W. *Comparison between the conventional and Bayesian approaches to evaluate measurement data.* Metrologia **43**, S249–S259 (2006).
23. International Organization for Standardization. *International vocabulary of metrology—Basic and general concepts and associated terms (VIM).* ISO/IEC Guide 99 (Geneva: ISO) (2008) and JCGM 200:2008. www.bipm.org/utils/common/documents/jcgm/JCGM_200_2008.pdf. Last accessed on June 13 2009.
24. International Organization for Standardization. *Statistics—vocabulary and symbols—Part 1: General statistical terms and terms used in probability.* ISO 3534-1 (Geneva: ISO) (2006).
25. Deutsches Institut für Normung. *Stochastik*. DIN 13303, Parts 1 and 2 (Berlin: Beuth) (1982) (in German).
26. Deutsches Institut für Normung. *Begriffe der Qualitätssicherung und Statistik (concepts of quality assurance and statistics)*. DIN 55350, Parts 21 to 24 (Berlin: Beuth) (1982 to 1987) (in German).
27. Press, W. H., Teukolsky, S. A., Vetterling, W. T. and Flannery, B. P. *Numerical Recipes in FORTRAN*, second edn. (Cambridge: Cambridge Unversity Press) (1992). Third edn. (2007) available.
28. Blanchard, P. and Brüning, E. Variational methods in mathematical physics (Berlin: Springer-Verlag) (1992).
29. Miller, G., Inkret, W. C., Schillaci, M. E., Martz, H. F. and Little, T. T. *Analyzing bioassay data using Bayesian methods—a primer. Bayesian prior probability distributions for internal dosimetry.* Health Phys. **78**, 598–613 (2000).

30. Weise, K. *Mathematical foundation of an analytical approach to Bayesian-statistical Monte Carlo spectrum unfolding*. PTB Report N–24 (Braunschweig: Physikalisch-Technische Bundesanstalt) (1995).
31. Cox, M., Forbes, A., Harris, P. and Sousa, J. *Accounting for physical knowledge in obtaining measurement results and associated uncertainties*. XVIII IMEKO World Congress. Metrology for a sustainable development (Rio de Janeiro) (2006).
32. Metropolis, N. A., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H. and Teller, E. *Equation of state calculation by fast computing machines*. J. Chem. Phys. **21**, 1087–1092 (1953).
33. Mackay, D. *Information theory, inference, and learning algorithms*, Chapter 29 (Cambridge: Cambridge University Press) (2003). www.inference.phy.cam.ac.uk/mackay/itila. Last accessed on June 13 2009.
34. Abramowitz, M. and Stegun, I. A. *Handbook of Mathematical Functions*, fifth edn. (New York: Dower Publications) (1968).
35. Weise, K. and Zhang, H. *Uncertainty treatment in Monte Carlo simulation*. J. Phys. A: Math. Gen. **30**, 5971–5980 (1997).
36. Gradshteyn, I. S. and Ryzhik, I. M. *Table of integrals, series, and products*, fourth edn. (New York, London: Academic Press) (1965).
37. Marsaglia, G. and Tsang, W. W. *A simple method for generating gamma variables*. ACM Trans. Math. Software **26**, 363–372 (2000).
38. Weise, K. and Wöger, W. *Removing model and data non-conformity in measurement evaluation*. Meas. Sci. Technol. **11**, 1649–1658 (2000).

APPENDIX 1: EXAMPLES OF THEORETICAL MC PREPARATION

Every MC application to a measurement requires a preceding theoretical preparation on the metrological level. Since counting measurement and spectrum unfolding play a dominant part in measurement of ionising radiation, they are chosen as examples to illustrate such preparations.

Counting measurement

Let N be a Poisson-distributed random counting variable with the parameter ϱt where $\varrho > 0$ is the count rate parameter and the constant t is the duration of a counting measurement with n events recorded. The random variable N follows a frequency distribution with the probability function (likelihood; not a density, see text below equation (18))

$$f_N(n \mid \varrho) = \Pr(N = n \mid R = \varrho) = \frac{(\varrho t)^n \mathrm{e}^{-\varrho t}}{n!}. \quad \text{(A.1)}$$

In BS, ϱ is taken as the value of a non-negative random variable R assigned to the count rate, acting here as the measurand to be determined. In order to obtain the distribution $f_R(\varrho \mid n)$ of R, the Bayes theorem is applied. It reads

$$f_R(\varrho \mid n) f_N(n) = f_N(n \mid \varrho) f_R(\varrho). \quad \text{(A.2)}$$

Here, $f_N(n)$ is a constant since n is given and $f_R(\varrho)$ is the *prior* of R, the distribution of R representing the information about R before the counting measurement is carried out. Mathematically, $f_R(\varrho)$ should be proportional to $1/\varrho$ because of a scale invariance with respect to the time[17]. But in the physical reality, there are often disregarded influences that could better be taken into account as a whole by setting $f_R(\varrho) \sim H(\varrho t)$, i.e. uniform for $\varrho \geq 0$[17]. The influences are caused, for instance, by dead-time and mean-life effects, pile-up of pulses, instrumental instabilities or by the choice of the duration t such that at least one event should be expected. With equation (A.1) and the uniform prior of R after a normalisation, equation (A.2) now yields

$$f_R(\varrho \mid n) = \frac{H(\varrho t) \cdot t\, (\varrho t)^n \mathrm{e}^{-\varrho t}}{\Gamma(n+1)}. \quad \text{(A.3)}$$

Accordingly, the count rate R with the value ϱ follows a gamma distribution with the expectation $\mathrm{E}(R \mid n) = r = (n+1)/t$ and the variance $\mathrm{Var}(R \mid n) = r/t = (n+1)/t^2$. The gamma function $\Gamma(n+1) = n!$ is used in equation (A.3) since n in general is not a natural number when the decision threshold and the detection limit are to be determined. The distribution can be transformed by the substitution $R = -(1/t)\ln Q$ into the finite region of Q with values q $(0 < q \leq 1)$ leading to $f_Q(q \mid n) = (-\ln q)^n/\Gamma(n+1)$. The standardised gamma distribution converges for $n \to \infty$ and fixed t *in distribution* to the standardised Gaussian normal distribution[17]. If, moreover, $t \to \infty$ but r remains finite, then the gamma distribution tends via the Gaussian distribution to the delta distribution $\delta(\varrho - r)$. The distribution function of R is an incomplete gamma function[27,34,36]. Convergence in distribution means—if some conditions are met—not only the pointwise convergence of a distribution to a limiting one but also that any intergral of a function formed with respect to the distribution converges to the corresponding integral with respect to the limiting distribution[17].

A sample ϱ from the gamma distribution according to equation (A.3) can be formed with $n+1$ standard random numbers $\theta_i > 0$ $(i = 1, \ldots, n+1)$[21]:

$$\varrho = -\frac{1}{t} \ln \left(\prod_{i=1}^{n+1} \theta_i \right). \quad \text{(A.4)}$$

This way of sampling can be modified if n is not a

natural number: Let $n = m + \lambda$ where m is a natural number and $0 < \lambda < 1$. For any integral with the gamma distribution involved, the obvious identity

$$\int L(\xi)\,\frac{\xi^n \mathrm{e}^{-\xi}}{\Gamma(n+1)}\,\mathrm{d}\xi = \int (L(\xi)\,\xi^{\lambda})\,\frac{\xi^m \mathrm{e}^{-\xi}}{\Gamma(m+1)}\,\mathrm{d}\xi \cdot \frac{\Gamma(m+1)}{\Gamma(m+\lambda+1)} \tag{A.5}$$

applies. Thus, equation (A.4) can be used with m instead of n and $L(\xi)\xi^{\lambda}$ instead of the arbitrary function $L(\xi)$. A sufficient approximation of the constant in equation (A.5) is

$$\frac{\Gamma(m+1)}{\Gamma(m+\lambda+1)} = (m+1)^{-\lambda} \times \left(1 + \frac{\lambda(1-\lambda)}{2(m+1)} + \frac{\lambda(1-\lambda^2)(2-3\lambda)}{24(m+1)^2} + \cdots\right) \tag{A.6}$$

based on reference[34]. The sampling described is not very practical for large n. Importance sampling then could be more suitable with $f_Q(q \mid n)$ since only values $q \approx 0$ can contribute considerably to an integral. For sampling from the gamma and Gaussian distributions, see also references[27,37].

The following subscripts g and 0 refer to independent counting radiation measurements of the gross and the background effects, respectively. The model $Y = G(\mathbf{X}) = X_1 - X_2 = R_g - R_0$ is introduced where $Y = R_n$ is the net count rate and $X_1 = R_g$ and $X_2 = R_0$. The set $\mathbf{a}$ consists of the recorded counts n_g and n_0 and of the measurement durations t_g and t_0, i.e. $\mathbf{a} = \{n_g, n_0, t_g, t_0\}$. The due rate values are $x_1 = \mathrm{E}(R_g \mid n_g) = r_g = (n_g + 1)/t_g$ and $x_2 = \mathrm{E}(R_0 \mid n_0) = r_0 = (n_0 + 1)/t_0$. A primary estimate of the measurand is $y_0 = x_1 - x_2 = r_g - r_0$. According to equation (3), all this yields

$$f_Y(y \mid \mathbf{a}) = \int \delta(y - \xi_1 + \xi_2) \times f_{X_1}(\xi_1 \mid n_g, t_g) f_{X_2}(\xi_2 \mid n_0, t_0)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2 = \int_0^{\infty} f_{X_1}(y + \xi \mid n_g, t_g) f_{X_2}(\xi \mid n_0, t_0)\,\mathrm{d}\xi. \tag{A.7}$$

This distribution is thus obtained by folding two gamma distributions. It also becomes a Gaussian distribution for large n_g, n_0, t_g, t_0 when standardised, since folding two Gaussian distributions again yields such a distribution.

In order to obtain $\widetilde{\mathbf{a}}(\widetilde{y})$ if n_g is missing before the gross-effect measurement is carried out, the model equation $\widetilde{y} = x_1 - x_2 = r_g - r_0$ is solved for $x_1 = r_g = \widetilde{y} + r_0$. This leads to $\widetilde{\mathbf{a}}(\widetilde{y})$ and to $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ by replacing n_g in $\mathbf{a}$ and in equation (A.7) by $(\widetilde{y} + r_0)t_g - 1$. The gamma distribution of $X_1 = R_g$ accordingly changes but the new value n_g is no longer necessarily a natural number. The model $Y = R_n = R_g - R_0$ just described is the simplest possible non-trivial model in measurement of ionising radiation.

When, for instance, a surface activity concentration is to be measured by the wipe test (see Appendix 3), additional input quantities are involved as, among others, the wiping efficiency X_3 with possible true values between c_0 and c_1 $(0 < c_0 < c_1 \leq 1)$. If nothing more is known of X_3, then, according to the PME, $f_{X_3}(\xi \mid c_0, c_1) = H(\xi - c_0)H(c_1 - \xi)/(c_1 - c_0)$ is a uniform distribution between c_0 and c_1. Moreover, $\mathbf{a} = \{n_g, n_0, t_g, t_0, c_0, c_1\}$. With the non-linear model equation $Y = G(\mathbf{X}) = (X_1 - X_2)/X_3$, the distribution

$$f_Y(y \mid \mathbf{a}) = \int \delta\left(y - \frac{\xi_1 - \xi_2}{\xi_3}\right) f_{X_1}(\xi_1 \mid n_g, t_g) \times f_{X_2}(\xi_2 \mid n_0, t_0) f_{X_3}(\xi_3 \mid c_0, c_1)\,\mathrm{d}\boldsymbol{\xi} \tag{A.8}$$

is obtained according to equation (3). It differs substancially from the Gaussian distribution if c_0 is a small value. Its expectation is $\mathrm{E}(Y \mid \mathbf{a}) = (r_g - r_0) \times \ln(c_1/c_0)/(c_1 - c_0)$. This expectation should not be confused with the best estimate $\widehat{y} = \mathrm{E}(Y \mid \mathbf{a}, y \geq 0)$ of the measurand according to equation (6).

$\widetilde{\mathbf{a}}(\widetilde{y})$ is obtained again by solving the model equation $\widetilde{y} = (x_1 - x_2)/x_3 = (r_g - r_0)/x_3$ for $x_1 = r_g = \widetilde{y}x_3 + r_0$. This leads to $\widetilde{\mathbf{a}}(\widetilde{y})$ and $f_Y(y \mid \widetilde{\mathbf{a}}(\widetilde{y}))$ by replacing n_g in $\mathbf{a}$ and equation (A.8) by $(\widetilde{y}x_3 + r_0)t_g - 1$. The expectation $\mathrm{E}(Y \mid \widetilde{\mathbf{a}}(\widetilde{y})) = \widetilde{y}x_3 \cdot \ln(c_1/c_0)/(c_1 - c_0)$ of this distribution should equal $\widetilde{y}$ according to equation (13). This condition finally yields $x_3 = (c_1 - c_0)/\ln(c_1/c_0)$.

Linear spectrum unfolding

A measured multi-channel spectrum with n_i events recorded in channel $i = 1, \ldots, \mu$ is to be unfolded. To each of the channels, a random variable $X_i = R_i$ is assigned which follows a gamma distribution $f_{X_i}(\xi_i \mid n_i)$ with $\xi_i = \varrho_i$ as in equation (A.3) of the preceding example and with $r_i = (n_i + 1)/t$. These input variables $\mathbf{X}$ are independent according to the PME if no further information about them is available. Let $\mathbf{a} = \{\mathbf{n}, t\}$. Then, $f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a}) = \prod_{i=1}^{\mu} f_{X_i}(\xi_i \mid n_i)$.

The set $\mathbf{a}$ can alternatively be expressed with $x_i = r_i$ by the column matrix $\mathbf{a} = \mathbf{x} = \mathbf{r}$ of the expectations of the input variables $\mathbf{X}$ or by the diagonal uncertainty (covariance) matrix $\mathbf{a} = \mathbf{U_x}(\mathbf{x}) = \mathrm{diag}(\mathbf{x})/t$, which is thus introduced as a function of $\mathbf{x}$ but with the fixed given data $\mathbf{x}$ of the immediate spectrum measurement inserted.

The measurand $Y = Y_1$ in question is the intensity of a particular spectral line of interest with the known shape $\psi_1(\vartheta)$ of the spectral density. ϑ is the variable assigned to the channel number, for instance, the time or the particle energy, $\vartheta = \vartheta_i$ for channel i with the width $\Delta\vartheta_i$. For the unfolding, the spectrum is expanded by this line and a suitable number $\nu - 1$ $(\nu < \mu)$ of background spectral-density components with shapes $\psi_k(\vartheta)$ $(k = 2, \ldots, \nu)$ including other lines, which may interfere. This is done by fitting a column matrix $\mathbf{z}$ to $\mathbf{x}$ with

$$z_i = \sum_{k=1}^{\nu} \psi_k(\vartheta_i)\Delta\vartheta_i \cdot y_k \quad \text{or} \quad \mathbf{z} = \mathbf{A}\mathbf{y} \tag{A.9}$$

by minimising $\chi^2 = (\mathbf{x} - \mathbf{z})^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{x})(\mathbf{x} - \mathbf{z})$. The constant matrix $\mathbf{A} = (A_{ik}) = (\psi_k(\vartheta_i)\Delta\vartheta_i)$ is called the spectrometer response matrix. The result of the fit is[2].

$$\begin{aligned} &\mathbf{y} = \mathbf{B}\mathbf{x}; \quad \mathbf{B} = \mathbf{U_y}\mathbf{A}^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{x}); \\ &\mathbf{U_y} = (\mathbf{A}^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{x})\mathbf{A})^{-1}. \end{aligned} \tag{A.10}$$

Equation (A.10) is now used to form the linear model equation $\mathbf{Y} = \mathbf{G}(\mathbf{X}) = \mathbf{B}\mathbf{X}$. Like $\mathbf{U_x}(\mathbf{x})$, the matrix $\mathbf{B}$ is taken as constant with the known fixed value $\mathbf{x}$. Then, $\mathbf{y}$ is also fixed, and it is analogous to the primary estimate y_0. According to equation (3), the distribution of $Y = Y_1$ then reads (η replaces y to avoid confusion with $\mathbf{y}$)

$$f_Y(\eta \,|\, \mathbf{a}) = \int \delta(\eta - (\mathbf{B}\boldsymbol{\xi})_1) \prod_{i=1}^{\mu} f_{X_i}(\xi_i \,|\, n_i) \mathrm{d}\xi_i. \tag{A.11}$$

This is nearly a Gaussian distribution with the expectation and, identically, the primary estimate $\mathrm{E}(Y \,|\, \mathbf{a}) = y_0 = y_1 = (\mathbf{B}\mathbf{x})_1$ and the variance $u^2(y_0) = (\mathbf{U_y})_{11}$ since y_0 and $u(y_0)$ remain finite if $\mu \to \infty$ as is shown in the following. In the case of a large μ, it is therefore not necessary to use MC, the application of ISO/FDIS 11929[2] is sufficient. Let the same spectrum be measured again with more and more channels but a fixed t. Then, essentially, $\Delta\vartheta_i$, $\mathbf{A}$ and $\mathbf{x}$ are $\sim 1/\mu$ and the diagonal matrix $\mathbf{U}_\mathbf{x}^{-1}(\mathbf{x})$ is $\sim\mu$. Accordingly, each of the $\nu \times \mu$ elements of $\mathbf{A}^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{x})$ is a product of a value $\sim 1/\mu$ times a value $\sim\mu$ and, thus, independent of μ. Similarly, each of the $\nu \times \nu$ elements of $\mathbf{A}^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{x}) \cdot \mathbf{A}$ is a sum of μ products of a value independent of μ times a value $\sim 1/\mu$ and is, therefore, also independent of μ. Hence it follows that $\mathbf{U_y}$ is also essentially independent of μ and remains finite. The same applies to the $\nu \times \mu$ elements of $\mathbf{B}$. Each of the ν elements of $\mathbf{y} = \mathbf{B}\mathbf{x}$ is then a sum of μ products of a value independent of μ times a value $\sim 1/\mu$ and is thus independent of μ and remains finite.

The model and the data conform if the chi-square criterion $|\min \chi^2 - (\mu - \nu)| \leq k\sqrt{2(\mu - \nu)}$ is met. k is an agreed factor preferably valued between 1 and 3. The applied minimum chi-square (also called the generalised least-squares) fit method turns out to be the only adjustment method satisfying the metrological requirements of a unique solution and a consistent uncertainty analysis in accordance with GUM[1]. Information conservation is a particular case of consistency. This feature and the fit method follow from the inherent symmetry of the suitably linearised model and of the information given by the measurement data and the associated uncertainties[38]. Additional information not taken into account by GUM, e.g. on non-negativity of quantities, can break the symmetry.

In order to finally obtain the set $\widetilde{\mathbf{a}}(\widetilde{y})$, the estimate y_1 of the measurand Y_1 in question is replaced by $\widetilde{y}$ leading to $\mathbf{y}' = (\widetilde{y}, y_2, \ldots)^\top$ and $\mathbf{z}' = \mathbf{A}\mathbf{y}'$. This $\mathbf{z}'$ is then used to replace $\mathbf{x}$ in equation (A.10) yielding $\widetilde{\mathbf{a}}(\widetilde{y}) = \mathbf{U_x}(\mathbf{A}\mathbf{y}') = \mathrm{diag}(\mathbf{A}\mathbf{y}')/t$ and $\mathbf{U}'_\mathbf{y} = (\mathbf{A}^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{A}\mathbf{y}')\mathbf{A}))^{-1}$. The distribution $f_Y(\eta \,|\, \widetilde{\mathbf{a}}(\widetilde{y}))$ then follows from equation (A.11) by accordingly replacing $\mathbf{B}$ by $\mathbf{B}' = \mathbf{U}'_\mathbf{y}\mathbf{A}^\top \mathbf{U}_\mathbf{x}^{-1}(\mathbf{A}\mathbf{y}')$. See also the next paragraph below equation (A.7) for the input gamma distributions changed accordingly.

APPENDIX 2: ILLUSTRATIVE NUMERIC EXAMPLE

To illustrate the distinctions between the usual Gaussian approach to the characteristic limits according to ISO/FDIS 11929[2] and the analytical and MC approaches, the already studied simplest realistic model $Y = X_1 - X_2$ in measurement of ionising radiation is chosen where the measurand Y is the difference of two count rates. Moreover, simple data cases as may occur in extremely low-level measurements are considered to make the distinctions quite obvious. With the Gaussian and analytical approaches, the data results are stated with five digits on the right of the decimal point so that they can also be used for testing programs under development. With the MC approach, however, the results obtained from 10^6 samples can be stated with an accuracy of two or three significant digits only.

Model, input data and first results

In the simple model $Y = R_g - R_0$ under consideration, the radiation measurand $Y = R_n$ is the net count rate, the difference between the gross count rate $X_1 = R_g$ and the background count rate $X_2 = R_0$. Counts $n_g = n_0 = n$ and preselected measurement durations $t_g = t_0 = t$ are considered as the input data **a**. The probabilities $\alpha = \beta = \gamma = 0.05$ are specified. When t is enlarged in the following in order to make a measurement more accurate, then the count rates to be measured do not change. Therefore, the count rate values $r_g = r_0 = r$ are kept constant. Accordingly, n is also enlarged but is in general no longer a natural number.

With the estimates $r = (n + 1)/t$ (with subscripts g or 0) and the associated squared standard uncertainties $u^2(r) = r/t$ of the input count rates, the primary estimate $y_0 = r_g - r_0 = 0$ of the measurand and the associated standard uncertainty $u(y_0) = \sqrt{u^2(r_g) + u^2(r_0)} = \sqrt{r_g/t_g + r_0/t_0} = \sqrt{2r/t}$ are first obtained. Since n_g is not available when the decision threshold and the detection limit are to be determined, the measurand value $\tilde{y}$ is assumed and n_g is replaced in the present case by $t\tilde{y} + n_0$ because $\tilde{y}$ replaces $y_0 = (n_g + 1)/t_g - (n_0 + 1)/t_0$. Notice that n_g does not change its given value n_0 by this replacement if $\tilde{y} = 0$.

Gaussian approach according to ISO/FDIS 11929

The application of ISO/FDIS 11929 (Section 6)[2] is quite easy. $f_Y(y \mid \mathbf{a})$ is a Gaussian distribution with expectation y_0 and variance $u^2(y_0)$. The best estimate $\hat{y}$ and the associated standard uncertainty $u(\hat{y})$ of the measurand Y follow from equations (33) and (34) of reference[2] with $r = 2$ corresponding to $n = 1$ if $t = 1$ (the arbitrary time unit is dropped for convenience; $r = (n + 1)/t$ is used instead of $r = n/t$ in reference[2] to make the results of the different approaches comparable):

$$\hat{y} = y_0 + \frac{u(y_0)\,\varphi(y_0/u(y_0))}{\omega} = u(y_0)\sqrt{\frac{2}{\pi}} = \frac{1.59577}{\sqrt{t}};$$
$$u(\hat{y}) = \sqrt{u^2(y_0) - (\hat{y} - y_0)\hat{y}} = u(y_0)\sqrt{1 - \frac{2}{\pi}} = \frac{1.20562}{\sqrt{t}}. \tag{A.12}$$

Here, $\varphi(x) = \exp(-x^2/2)/\sqrt{2\pi}$ is the standardised Gaussian distribution, $\Phi(x)$ is its distribution function and $\omega = \Phi(y_0/u(y_0)) = 1/2$. Moreover, k_p is the p-quantile with $\Phi(k_p) = p$. The limits $y^{\triangleleft}$ and $y^{\triangleright}$ of the coverage interval are obtained from equations (29) to (31) of reference[2]. The results are $p = 0.4875$; $q = 0.9875$; $k_p = -0.03134$; $k_q = 2.24140$ and

$$y^{\triangleleft} = y_0 - k_p u(y_0) = \frac{0.06268}{\sqrt{t}};$$
$$y^{\triangleright} = y_0 + k_q u(y_0) = \frac{4.48281}{\sqrt{t}}. \tag{A.13}$$

The computation of the decision threshold y^* and the detection limit $y^\sharp$ requires the uncertainty function $\tilde{u}(\tilde{y}) = \sqrt{(\tilde{y} + r_0)/t_g + r_0/t_0}$ according to equation (14) of reference[2] (with $w = x_3 = 1$, $x_4 = 0$ and vanishing associated uncertainties). According to equation (13), the assumed true value $\tilde{y}$ and the squared uncertainty function $\tilde{u}^2(\tilde{y})$ are the expectation and the variance, respectively, of $f_Y(y \mid \tilde{\mathbf{a}}(\tilde{y}))$ which is here a Gaussian distribution. Here, $\tilde{u}^2(\tilde{y}) = c_0 + c_1\tilde{y} + c_2\tilde{y}^2$ with $c_0 = r_0(1/t_g + 1/t_0) = 4/t$; $c_1 = 1/t_g = 1/t$; $c_2 = 0$. Equations (21), (22), (27) and (28) of reference[2] then yield the following with $k = k_{1-\alpha} = k_{1-\beta} = 1.64485$ since $\alpha = \beta$ (see also Figure 2 and Figure A1):

$$y^* = k_{1-\alpha}\tilde{u}(0) = k\sqrt{c_0} = \frac{3.28971}{\sqrt{t}};$$
$$y^\sharp = y^* + k_{1-\beta}\tilde{u}(y^\sharp) = \frac{2y^* + k^2 c_1}{1 - k^2 c_2} = 2y^* + \frac{k^2}{t}$$
$$= \frac{6.57942}{\sqrt{t}} + \frac{2.70554}{t}. \tag{A.14}$$

This means $y^\sharp/(2y^*) = 1 + y^*/8 = 1 + 0.41121/\sqrt{t}$ (see Figure A2) and $y^\sharp = 9.28496$ for $t = 1$ and $y^\sharp = 0.68500$ for $t = 100$. See also the following MC approach subsection and Appendix 3 where the results of the Gaussian approach are marked by the subscript G.

Analytical approach

Only the case $n = 1$ and $t = 1$ is treated with the analytical approach. Otherwise, the complicated integrals involved would require an unreasonable amount of computation. The gamma distribution according to equation (A.3) then reads $f_R(\varrho \mid 1) = H(\varrho)\,\varrho\,\mathrm{e}^{-\varrho}$. By using this distribution in the folding integral of equation (A.7), the integration can be carried out and yields $f_Y(y \mid \mathbf{a}) = (1 + |y|)\mathrm{e}^{-|y|}/4$. The corresponding Gaussian distribution with the same expectation 0 and variance 4 has the shape $\exp(-y^2/8)/(2\sqrt{2\pi})$. Notice that for $y < 0$, the lower limit of the folding integral is $|y|$ instead of 0 since the integrand cannot be negative for it is a product of distributions. The distribution $f_Y(y \mid \mathbf{a}, y \geq 0) = H(y)(1 + y)\mathrm{e}^{-y}/2$ is obtained according to equation (4) by truncating $f_Y(y \mid \mathbf{a})$ at $y = 0$ and

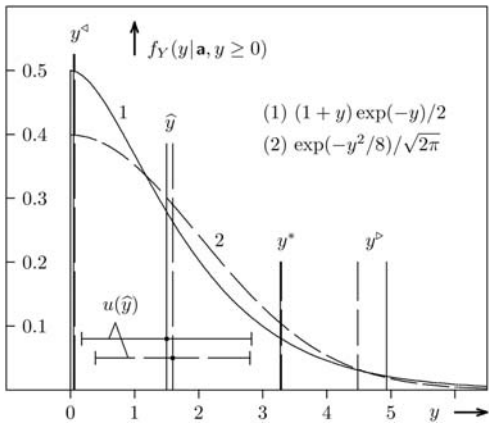

Figure A1. Comparison of two cases of the distribution of possible non-negative true measurand values y for the numeric example treated, of the best estimate $\widehat{y}$ (expectation) of the measurand Y with the associated standard uncertainty $u(\widehat{y})$ (standard deviation), and of the limits $y^{\triangleleft}$ and $y^{\triangleright}$ of the coverage interval. (1) Analytical approach, (2) Gaussian approach according to ISO/FDIS 11929[2] (dashed lines). The decision threshold values y^* can also be compared since the distributions $f_Y(y\,|\,\mathbf{a})$ and $f_Y(y\,|\,\widetilde{\mathbf{a}}(\widetilde{y}=0))$ are identical in the simple data case considered with $n=1$ event recorded in the gross and background measurements of duration $t=1$ (arbitrary time unit). The remarkable difference of the $y^{\triangleright}$ values is caused by the more pronounced distribution tail in case (1).

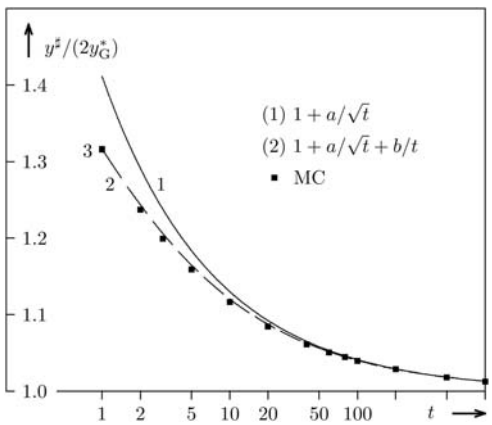

Figure A2. Detection limit $y^{\sharp}$ as a function of the measurement duration t of the numeric example treated. The double decision threshold $2y^*_G$ of the Gaussian case is used as the scaling function since, asymptotically for large t, it equals the detection limit. (1) Gaussian approach according to ISO/FDIS 11929[2] and equation (A.14) with $a=0.41121$. (2) Approximation of the analytical and MC approaches (dashed line). The coefficient $b=-0.09486$ is obtained by adaption to the analytical result (3) at $t=1$ according to equations (A.19) and (A.23). See the text for more details.

renormalising (see Figure A1). Its expectation and standard deviation are

$$\widehat{y}=\frac{3}{2};\quad u(\widehat{y})=\frac{\sqrt{7}}{2}=1.32288. \tag{A.15}$$

Quantiles are needed for the limits $y^{\triangleleft}$ and $y^{\triangleright}$ of the coverage interval. They are determined by means of the distribution function $F_Y(y\,|\,\mathbf{a}, y\geq 0)=1-(2+y)\mathrm{e}^{-y}/2$ obtained by integrating the distribution density from 0 to y. Equations (8) and (9) first yield the conditions:

$$\begin{aligned} 1-\frac{(2+y^{\triangleleft})\mathrm{e}^{-y^{\triangleleft}}}{2}&=\frac{\gamma}{2};\\ 1-\frac{(2+y^{\triangleright})\mathrm{e}^{-y^{\triangleright}}}{2}&=1-\frac{\gamma}{2}. \end{aligned} \tag{A.16}$$

Solving for the exponents leads to the following iteration equations and results

$$\begin{aligned} y^{\triangleleft}&=\ln\left(\frac{2+y^{\triangleleft}}{2-\gamma}\right)=0.05002;\\ y^{\triangleright}&=\ln\left(\frac{2+y^{\triangleright}}{\gamma}\right)=4.93186 \end{aligned} \tag{A.17}$$

by starting with suitable values, for instance, values 0. Equations (A.16) are not solved for the limits in the brackets since this would lead to divergent iterations. The decision threshold y^* can be obtained in a similar way. In order to determine the function $\widetilde{\mathbf{a}}(\widetilde{y})$, the gross-effect count number n_g has to be replaced by $(\widetilde{y}+r_0)t_g-1=1$ if $\widetilde{y}=0$. But n_g already equals 1. Therefore, the distributions $f_Y(y\,|\,\widetilde{\mathbf{a}}(\widetilde{y}=0))$ and $f_Y(y\,|\,\mathbf{a})=(1+|\,y\,|)\mathrm{e}^{-|y|}/4$ are in the present case identical and symmetric with respect to $y=0$. The integral of this distribution from $-\infty$ to $y\geq 0$ is the distribution function $FY(y\,|\,\widetilde{\mathbf{a}}(\widetilde{y}=0))=1-(2+y)\mathrm{e}^{-y}/4$. It equals 1/2 for $y=0$ since the distribution is even. Equation (10) now reads

$$1-\frac{(2+y^*)\mathrm{e}^{-y^*}}{4}=1-\alpha. \tag{A.18}$$

Solving for the exponent leads to the iteration equation and the decision threshold

$$y^*=\ln\left(\frac{2+y^*}{4\alpha}\right)=3.27181. \tag{A.19}$$

Not only the analytical but also the MC calculation of the detection limit $y^{\sharp}$ requires much more effort, mainly since the value $(\widetilde{y}+r_0)t_g-1=\widetilde{y}+1>1$ replacing n_g is in general no longer a natural number. The distribution function $F_Y(y\,|\,\widetilde{\mathbf{a}}(\widetilde{y}))$ is

needed, at least for $y \geq 0$, to obtain $y^\sharp$ from the condition $F_Y(y^* \,|\, \widetilde{\mathbf{a}}(\widetilde{y} = y^\sharp)) = \beta$ according to equation (11). It follows from equations (3) and (A.3):

$$F_Y(y \,|\, \widetilde{\mathbf{a}}(\widetilde{y})) = \frac{K}{\Gamma(\widetilde{y}+2)} \quad (y \geq 0) \tag{A.20}$$

with

$$\begin{aligned} K &= \int_0^\infty \int_0^\infty H(y - \xi_1 + \xi_2)\widetilde{\xi_1^{y+1}} \mathrm{e}^{-\xi_1} \xi_2 \mathrm{e}^{-\xi_2} \mathrm{d}\xi_1 \mathrm{d}\xi_2 \\ &= \int_0^\infty \left(\int_{\max(0,\xi_1 - y)}^\infty \xi_2 \mathrm{e}^{-\xi_2} \mathrm{d}\xi_2 \right) \widetilde{\xi_1^{y+1}} \mathrm{e}^{-\xi_1} \mathrm{d}\xi_1 \\ &= \int_0^\infty (\max(0, \xi - y) + 1)\widetilde{\xi^{y+1}} \\ &\quad \times \exp(-\xi - \max(0, \xi - y))\mathrm{d}\xi \\ &= \int_0^y \widetilde{\xi^{y+1}} \mathrm{e}^{-\xi} \mathrm{d}\xi + \int_y^\infty (\xi - y + 1)\widetilde{\xi^{y+1}} \mathrm{e}^{-2\xi + y} \mathrm{d}\xi \\ &= \Gamma(\widetilde{y}+2) - \Gamma(\widetilde{y}+2, y) + \frac{\mathrm{e}^y}{2^{\widetilde{y}+3}} \\ &\quad \times (\Gamma(\widetilde{y}+3, 2y) - 2(y-1)\Gamma(\widetilde{y}+2, 2y)). \end{aligned} \tag{A.21}$$

The subscript 1 is dropped. $\Gamma(a, x) = \int_x^\infty \xi^{a-1} \mathrm{e}^{-\xi} \mathrm{d}\xi$ is an incomplete gamma function[27,34,36]. Equation (A.21) applies only for $y \geq 0$. For $y = 0$, the distribution function has the particular value $F_Y(0 \,|\, \widetilde{\mathbf{a}}(\widetilde{y})) = (\widetilde{y}+4)/2^{\widetilde{y}+3}$. By introducing $Q(a,\ x) = \Gamma(a,\ x)/\Gamma(a)$ and using the well-known recurrence formula $\Gamma(a+1) = a\Gamma(a)$ for $a = \widetilde{y}+2$, finally

$$\begin{aligned} F_Y(y \,|\, \widetilde{\mathbf{a}}(\widetilde{y})) &= 1 - Q(\widetilde{y}+2, y) + \frac{\mathrm{e}^y}{2^{\widetilde{y}+3}} \\ &\quad \times \Big((\widetilde{y}+2) Q(\widetilde{y}+3, 2y) \\ &\quad - 2(y-1) Q(\widetilde{y}+2, 2y) \Big). \end{aligned} \tag{A.22}$$

is obtained. A subroutine for a numeric calculation of $Q(a,x)$ is provided by reference [27]. The result

$$y^\sharp = 8.66083 \tag{A.23}$$

for the detection limit is found by varying $\widetilde{y}$ until the distribution function assumes the value β.

The results according to equations (A.15), (A.17), (A.19) and (A.23) should be compared with those according to equations (A.12)–(A.14) of the Gaussian approach with $t = 1$.

MC approach

The results of equations (A.15), (A.17) and (A.19) could easily be verified with an accuracy of at least two or three significant digits by an MC run with $N = 10^6$ samples drawn by means of equation (A.4). A computing time of a few seconds per MC run was needed on a moderately fast personal computer. Not only the measurement duration $t = 1$ was considered, but also 12 other values up to $t = 1000$ (see Figure A2). In the case of the detection limit, equation (A.4) could not be used directly since $n_\mathrm{g} = \widetilde{y} + 1$ is then in general not a natural number. Instead, the result was obtained by applying the modified sampling according to equations (A.4)–(A.6) with $n = n_\mathrm{g} = \widetilde{y} + 1 = m + \lambda$. Random-number generators for the gamma distribution from references [27,37] were also used.

Let $y^\bullet$ be any one of $\widehat{y}, u(\widehat{y}), y^\triangleleft, y^\triangleright, y^*, y^\sharp$ and $y^\sharp/(2y_\mathrm{G}^*)$ and, moreover, $y_\mathrm{G}^\bullet$ be that $y^\bullet$ obtained by the Gaussian approach. Then the following empirical approximations turn out to have in the considered data case a sufficiently large accuracy for every t:

$$y^\bullet \approx y_\mathrm{G}^\bullet + \frac{c}{t}; \quad c = y^\bullet \,|_{t=1} - y_\mathrm{G}^\bullet \,|_{t=1}. \tag{A.24}$$

The values on the right-hand sides of equation (A.24) are given by equations (A.12)–(A.15), (A.17), (A.19) and (A.23). MC is not involved.

As an example of the dependence of the results on the measurement duration t, values $y^\sharp/(2y_\mathrm{G}^*)$ are shown in Figure A2. Here, the double decision threshold $2y_\mathrm{G}^*$ is used as the scaling function since, asymptotically for large t, it equals the detection limit $y^\sharp$. The corresponding plots for all the $y^\bullet$ look quite similar. There are small systematic differences between the values $y^\bullet$ according to equation (A.24) and the MC results $y_\mathrm{MC}^\bullet$. They are obvious for small $t <\approx 20$, but disappear for large t, and have for each $y^\bullet$ at $t \approx 5$ their maximum of $|y^\bullet - y_\mathrm{MC}^\bullet|/y_\mathrm{MC}^\bullet <\approx 2.2\,\%$, in particular, $\approx 0.4\,\%$ for $y^\sharp/(2y_\mathrm{G}^*)$, and with the exception of $\approx 5.5\,\%$ for $y^\triangleleft$.

The term c/t in equation (A.24) and the mentioned systematic differences can be caused by terms of higher order in $1/\sqrt{t}$ represented by the correction terms and the dots following the leading Gaussian terms in equations (A.36)–(A.40) with $t \sim \tau$ and $b_3 = 0$. Although the two correction terms in equation (A.37) disappear rapidly with $\tau \to \infty$, they can contribute appreciably for smaller t or τ to deviations from the Gaussian case.

For all the considered values of t, the relative MC-induced uncertainties $u_\mathrm{MC}(y^\bullet)/y^\bullet <\approx 2.4 \times 10^{-3}$ were obtained in the same order of magnitude according to equation (40) with $\nu = 20$ independent

MC runs. As an exception, the rather small $y^{\triangleleft}$ has a relative MC-induced uncertainty $<\approx 1.2 \times 10^{-2}$.

APPENDIX 3: PROBLEMS IN MC APPLICATION

Some typical problems are involved in the application of the MC method in the practice of ionising-radiation measurement. Four of them are treated in the following. They can occur already with the simple wipe test in radiation protection and are caused by

(a) an MC-statistical divergence,
(b) a strongly non-linear model function,
(c) using a Gaussian instead of a gamma distribution,
(d) a non-existent detection limit.

MC-statistical divergence

In many cases, the MC approach does not converge. This can be caused by a non-negative input quantity X, which occurs reciprocally in the model function G and can assume the value $\xi = 0$. The expectation of $1/X$ then does not exist. Examples are the denominator quantities $X_5, X_7, \ldots$ of the model equation

$$Y = (X_1 - X_2X_3 - X_4) \cdot \frac{X_6X_8 \ldots}{X_5X_7 \ldots} \qquad \text{(A.25)}$$

which is often appropriate in ionising-radiation measurement and is therefore treated in ISO/FDIS 11929[2]. A simple truncation of the distribution $f_X(\xi)$ at $\xi = 0$ does not remove the divergence. Then an attempt has to be made to truncate $f_X(\xi)$ at a reasonably assessed value $\xi > 0$. This can be done, for instance, by replacing the distribution by a uniform distribution with the same expectation and variance, provided that the standard uncertainty of X is small enough so that the lower bound of the uniform distribution is positive.

This advice may seem somewhat arbitrary since, according to the PME, a Gaussian distribution should be assigned to X if only an estimate x and the associated standard uncertainty $u(x)$ are known. But often there is much more, still unused information from previous measurements, experience or elsewhere that can justify a reasonable truncation of the distribution at a positive value of X. This is allowed in BS and is similar to using a more realistic uniform count rate prior in Appendix 1 instead of a theoretical prior proportional to the reciprocal count rate. Nevertheless, if the distribution $f_X(\xi)$ is not truncated and samples $\xi < 0$ are admitted, then, remarkably, the expectation $\mathrm{E}(1/X)$ exists as a principal integral value since

$$\int_{-a}^{a} \frac{f_X(\xi)}{\xi} \mathrm{d}\xi = 2af'_X(0) + \frac{a^3}{9} f'''_X(0) + \cdots \qquad \text{(A.26)}$$

with some a by using a Taylor expansion of the distribution at $\xi = 0$. The integral is very small in the case of the Gaussian distribution if $x \gg u(x)$. But the MC-induced uncertainty u_{MC} associated with $\mathrm{E}(1/X)$ turns out to be infinite according to equation (25) since the integral $\int_{-a}^{a} L^2(\xi)\mathrm{d}\xi$ for $L(\xi) = f_Y(\xi)/\xi$ in most cases does not exist. Finally, it should be noted that even with a truncated distribution of X, the distribution of $1/X$ and, as a consequence, also the distribution of Y according to equation (A.25), can show pronounced upper tails.

Strongly non-linear model function

There are other cases where the results obtained from a convergent MC approach can differ significantly from those of the Gaussian approach because of a strongly non-linear model function or non-Gaussian distributions of a few input quantities. To avoid such cases in practice, the measurement procedure should be inspected. The input quantities causing the problem often have relatively large uncertainties. An attempt should be made to improve the accuracy in the measurements of these quantities.

An example is again a factor $1/X$ as in equation (A.25) with a given value x and standard uncertainty $u(x)$ of X. Then, $1/x$ is inserted with the ISO/FDIS 11929 approach in contrast to

$$\mathrm{E}\left(\frac{1}{X}\right) = \frac{1}{2\delta} \ln\left(\frac{x+\delta}{x-\delta}\right) = \frac{1}{x}\left(1 + \frac{u^2(x)}{x^2} + \cdots\right); \quad \delta = u(x)\sqrt{3} \qquad \text{(A.27)}$$

with the MC approach if a uniform distribution is assigned to X with the expectation x, the variance $u^2(x)$, the width 2δ, and $x - \delta > 0$. The smaller $u(x)$, the more the two compared values $1/x$ and $E(1/X)$ agree.

Gaussian approximation of a gamma distribution

The gamma distribution plays a dominant part in counting radiation events (see Appendix 1). But MC count rate sampling according to equation (A.4) is not very practical for a large number n of counts. Although the standardised gamma distribution is known to converge (in distribution) to the standardised Gaussian distribution with $n \to \infty$[17], the questions remain of how fast this convergence is and what the consequences are when the gamma distribution is approximated by the Gaussian one. To investigate these questions, the model equation $Y = X_1 - X_2 = R_g - R_0$ is again considered as in Appendix 1. The distribution $f_Y(y \mid \mathbf{a})$ is then given according to equation (A.7) and the gamma

distributions of the count rates $X_1 = R_g$ and $X_2 = R_0$ according to equation (A.3).

Any distribution $f(y)$, which is to be approximated by the Gaussian distribution $f_G(y) = \exp(-\zeta^2/2)/\sqrt{2\pi\sigma^2}$—where $\zeta = (y-\mu)/\sigma$ and both distributions have the same expectation μ and variance σ^2 – can be expanded in a series of Hermite polynomials $He_k(\zeta)$[34] used and defined by

$$f(y) = f_G(y)\sum_{k=0}^{\infty}\frac{a_k}{k!}He_k(\zeta);$$
$$He_k(\zeta) = (-1)^k e^{\zeta^2/2}\frac{d^k e^{-\zeta^2/2}}{d\zeta^k}. \tag{A.28}$$

The defining equation is called the Rodrigues formula. The Hermite polynomials meet the orthogonality relations

$$\int_{-\infty}^{\infty} e^{-\zeta^2/2}He_j(\zeta)He_k(\zeta)d\zeta = \begin{cases} 0 & (j \neq k) \\ \sqrt{2\pi}\cdot j! & (j = k). \end{cases} \tag{A.29}$$

In particular, $He_0(\zeta) = 1, He_1(\zeta) = \zeta$, $He_2(\zeta) = \zeta^2 - 1, He_3(\zeta) = \zeta^3 - 3\zeta$ and $He_4(\zeta) = \zeta^4 - 6\zeta^2 + 3$. The coefficients a_j are obtained by multiplying the series in equation (A.28) by $He_j(\zeta)$, integrating, and using the orthogonality relations. This yields

$$a_j = \sigma\int_{-\infty}^{\infty}He_j(\zeta)f(y)d\zeta = \int_{-\infty}^{\infty}He_j\left(\frac{y-\mu}{\sigma}\right)f(y)dy. \tag{A.30}$$

In particular, $a_0 = 1$, $a_1 = a_2 = 0$, the skewness $a_3 = \mu_3/\sigma^3$ and the excess $a_4 = \mu_4/\sigma^4 - 3$ of the distribution $f(y)$ follow where $\mu_j = E((Y-\mu)^j)$ is the jth central moment of $f(y)$. If $f(y)$ is symmetric with respect to $y = \mu$, then $a_j = 0$ for all odd j. Finally,

$$f(y) = f_G(y)\left(1 + \frac{a_3}{3!}He_3(\zeta) + \frac{a_4}{4!}He_4(\zeta) + \cdots\right) \tag{A.31}$$

The distribution $f_Y(y\,|\,\mathbf{a})$ of $Y = R_g - R_0$ according to equation (A.7) is now taken as $f(y)$. Its expectation $\mu = (n_g+1)/t_g - (n_0+1)/t_0 = r_g - r_0$ and variance $\sigma^2 = r_g/t_g + r_0/t_0$ are already known. Its skewness a_3 and excess a_4 are also needed to show the behaviour of the distribution for large numbers of recorded radiation events and measurement durations.

To this end, a gamma-distributed count rate R with the true value ϱ is first considered with a number n of counts recorded from a Poisson distribution during a measurement of duration t. The gamma distribution $f_R(\varrho\,|\,n,t)$ is given according to equation (A.3). The *characteristic function* of R then becomes

$$\begin{aligned}\phi_R(k) &= E(e^{ikR}) \\ &= \int_0^{\infty}\frac{(\varrho t)^n e^{-\varrho t\cdot(1-ik/t)}}{\Gamma(n+1)}d(\varrho t) \\ &= \frac{1}{(1-ik/t)^{n+1}}\end{aligned} \tag{A.32}$$

by substituting $v = \varrho t\cdot(1-ik/t)$. This leads to

$$\begin{aligned}\phi_Y(k) &= E(\exp(ik\cdot(R_g - R_0)) \\ &= \phi_{R_g}(k)\,\phi_{R_0}(-k)\end{aligned} \tag{A.33}$$

$$\begin{aligned}\ln\phi_Y(k) = &-(n_g+1)\ln(1-ik/t_g) \\ &-(n_0+1)\ln\frac{1+ik}{t_0} = \sum_{j=1}^{\infty}\kappa_j\frac{(ik)^j}{j!}\end{aligned} \tag{A.34}$$

$$\begin{aligned}\kappa_j &= (j-1)!\left(\frac{n_g+1}{t_g^j} + (-1)^j\frac{n_0+1}{t_0^j}\right) \\ &= (j-1)!\left(\frac{r_g}{t_g^{j-1}} + \frac{(-1)^j r_0}{t_0^{j-1}}\right)\end{aligned} \tag{A.35}$$

by expanding $\ln\phi_Y(k)$ in a power series of ik. The coefficients κ_j are the *cumulants* of Y. In particular, these are the expectation $\kappa_1 = \mu = r_g - r_0$, the variance $\kappa_2 = \sigma^2$, the skewness $\kappa_3/\kappa_2^{3/2} = \kappa_3/\sigma^3 = a_3$ and the excess $\kappa_4/\kappa_2^2 = \kappa_4/\sigma^4 = a_4$[34].

In order to make the measurement more accurate, the data n_g+1, n_0+1, t_g and t_0 are now enlarged proportionally to an increasing parameter τ such that r_g, r_0 and μ remain constant. Then, $\sigma^2 \sim 1/\tau, \kappa_j \sim 1/\tau^{j-1}, a_3 \sim 1/\sqrt{\tau}$ and $a_4 \sim 1/\tau$. Equation (A.31) finally becomes with some coefficients b_3 and b_4 independent of τ

$$f_Y(y\,|\,\mathbf{a}) = f_G(y)\left(1 + \frac{b_3}{\sqrt{\tau}}He_3(\zeta) + \frac{b_4}{\tau}He_4(\zeta) + \cdots\right) \tag{A.36}$$

Here, $f_G(y)$ represents the Gaussian distribution approximating $f_Y(y\,|\,\mathbf{a})$ and the large bracket is the correction factor, the second and all following terms of which vanish with the increasing τ. The dots stand for terms proportional to $\tau^{-\nu}$ with $\nu > 1$. The term with b_3 exactly vanishes for $b_3 = 0$, i.e. if $f_Y(y\,|\,\mathbf{a})$ has zero skewness $a_3 = 0$, for instance, if it is

symmetric with respect to the expectation μ as in the data case of Appendix 2. It is stressed that the statement according to equation (A.36) is not absolute but only shows how the distribution of Y is related to $f_G(y)$, which itself depends on τ since $\sigma^2 \sim 1/\tau$ and thus converges (in distribution) to the delta function $\delta(y—\mu)$ if $\tau \to \infty$.

Any type-A integral $I = \int_a^b g(y) f_Y(y \mid \mathbf{a}) \mathrm{d}y$ and the corresponding integral $I_G = \int_a^b g(y) f_G(y) \mathrm{d}y$ with the Gaussian distribution are now considered. Using equation (A.26) and assuming for $g(y)$ at $y = \mu$ with $y - \mu = \sigma\zeta$ a convergent Taylor series $g(y) = g(\mu) + \sigma g'(\mu)\zeta + \sigma^2 g''(\mu)\zeta^2/2 + \cdots$ yield

$$I = I_G + \frac{b_3}{\sqrt{2\pi\tau}} \int_{(a-\mu)/\sigma}^{(b-\mu)/\sigma} \mathrm{e}^{-\zeta^2/2} \left(g(\mu) + \sigma g'(\mu)\zeta\right) \times \mathrm{He}_3(\zeta)\mathrm{d}\zeta + \frac{b_4 g(\mu)}{\tau\sqrt{2\pi}} \int_{(a-\mu)/\sigma}^{(b-\mu)/\sigma} \mathrm{e}^{-\zeta^2/2} \mathrm{He}_4(\zeta)\mathrm{d}\zeta + \cdots \tag{A.37}$$

Both the correction terms on the right-hand side of equation (A.37) disappear for $\tau \to \infty$ not only because of τ in the denominators, but also since the integrals vanish if $a, b \neq \mu$. This follows with $\sigma \sim 1/\sqrt{\tau}$ and $1 = \mathrm{He}_0(\zeta)$ and $\zeta = \mathrm{He}_1(\zeta)$ from the orthogonality relations according to equation (A.29) since the integral limits tend to $\pm\infty$. Thus, if the correction terms are neglected or if $a = -\infty$ and $b = +\infty$, and with the Taylor series of $g(y)$, then

$$I = \mathrm{E}(g(Y)) = I_G + \cdots = g(\mu) + \frac{\sigma^2 g''(\mu)}{2} + \cdots \tag{A.38}$$

A type-B or type-C integral $I(\eta)$ depends on a parameter η to be determined from the equation $I(\eta) = p$ with a given integral value p. Let $I(\eta) = I_G(\eta) + \delta I(\eta)/\tau^\nu$ $(\nu > 0)$ and, moreover, η_G first obtained from $I_G(\eta_G) = p$. By expanding at η_G then

$$p = I(\eta) = I_G(\eta_G) + \frac{1}{\tau^\nu}\delta I(\eta_G) + \left(I'_G(\eta_G) + \frac{1}{\tau^\nu}\delta I'(\eta_G)\right)(\eta - \eta_G) + \cdots \tag{A.39}$$

follows. The dots refer to terms proportional to higher powers of $\eta - \eta_G$. Equation (A.29) is solved for η with $I(\eta) = I_G(\eta_G) = p$ and results in

$$\eta = \eta_G - \frac{\delta I(\eta_G)}{\tau^\nu I'_G(\eta_G)} + \cdots \tag{A.40}$$

Here, the dots also include terms proportional to $\tau^{-\nu'}$ with $\nu' > \nu$. The leading correction term is thus also proportional to $\tau^{-\nu}$. If a p-quantile η of a distribution $f(y)$ is to be determined, then $I'_G(\eta_G) = f_G(\eta_G)$.

Equations (A.36)–(A.40) also apply quite generally to any distribution $f_Y(y \mid \ldots) = f_G(y) + \delta f_Y(y \mid \ldots)/\tau^\nu$. See the MC subsection of Appendix 2 for numeric examples.

Non-existent detection limit

Sometimes, there is no detection limit $y^\sharp$. This can easily be seen in equation (A.14) cited from ISO/FDIS 11929[2]. If $k^2 c_2 \geq 1$, then a meaningless negative or infinite $y^\sharp$ is obtained and the measurement procedure tested is thus not suitable at all for the intended measurement purpose. $c_2 = u^2_{\mathrm{rel}}(w)$ is the squared relative standard uncertainty associated with the estimate w of the fraction, summarily denoted by W, in the model equation (A.25).

More efforts are required to verify the non-existence of $y^\sharp$ with the MC method. But if a guideline value y_r is given, then $y^\sharp$ is not always needed. It is sufficient that the condition $I_7 = P(y_r) \leq \beta$ is met for the decision that the measurement procedure is suitable (see equation (12) and the accompanying text). The type-A integral I_7 can easily be obtained by MC. If $I_7 \leq \beta$, then $y^\sharp$ exists. If $I_7 > \beta$, then $y^\sharp$ possibly also exists, but the measurement procedure is unsuitable. In addition, the shape of the function $P(\widetilde{y})$ must be analysed. A minimum greater than β will then give a strong indication that $y^\sharp$ does not exist. In this case, an attempt should be made to reduce by experimental means the uncertainties of the input quantities X_i contributing to the fraction W.

The wipe test as a problematic example

For the examination of surface contamination by means of the wipe test, the measurand Y is the surface activity concentration A_F (activity divided by the wiped area). For this task, the best estimate, the associated standard uncertainty and the characteristic limits are to be calculated according to ISO/FDIS 11929[2] and MC. The model equation in this case reads

$$Y = A_F = G(\mathbf{X}) = \frac{X_1 - X_2}{X_3 X_4 X_5} = \frac{\varrho_g - \varrho_0}{F\,\kappa\,\varepsilon}. \tag{A.41}$$

$X_1 = \varrho_g$ is the gross count rate and $X_2 = \varrho_0$ is the background count rate, $X_3 = F$ is the wiped area, $X_4 = \kappa$ is the detection efficiency and $X_5 = \varepsilon$ is the wiping efficiency, i.e. the fraction of the wipeable activity for the material of the surface to be examined.

After the counting measurements of the gross effect and of the background effect have been carried out with the respective measurement durations t_g and t_0, the respective numbers n_g and n_0 of the recorded radiation events are available. These numbers are used according to GUM[1] and ISO/FDIS 11929 to specify the estimates $x_1 = r_g = n_g/t_g$ with $u^2(x_1) = n_g/t_g^2 = r_g/t_g$ for the gross count rate $X_1 = \varrho_g$ 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 $X_2 = \varrho_0$. These specifications apply to measurements with time pre-selection. The uncertainties of the measurement durations are neglected since time can be measured much more accurately than any other physical quantity involved. Since the numbers of recorded events are large, the gamma distributions of the count rates are replaced by Gaussian distributions for the MC calculations. This causes problem (c).

The relative standard uncertainty of the wiped area F is given as 10% from experience, leading to $u(F) = 10\ \mathrm{cm}^2$. The detection efficiency κ 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, $u(\kappa) = 0.0155$ results. The quantities F and κ occur in the denominator of the model function G. Gaussian distributions therefore cannot be assigned to them because of problem (a). Instead, uniform distributions are used with the same respective expectations and standard deviations u leading to the width $\Delta = u\sqrt{12}$.

The wiping efficiency ε of the wipe test is known from previous measurements to be randomly distributed between 0.06 and 0.62. These bounds yield the mean estimate $\varepsilon = 0.34$ and the associated standard uncertainty $u(\varepsilon) = \Delta\varepsilon/\sqrt{12}$ since, according to the PME, a uniform distribution over the region of the possible values of ε with the width $\Delta\varepsilon = 0.56$ can be specified.

A more informative distribution function F_ε can be established if a pool of comparable wiping-efficiency data ε_k from the previous measurements is available. See paragraphs (c) and (d) of subsection 'Additional remarks' below equation (19).

For all the input data and results, see Table A1. The results are calculated according to ISO/FDIS 11929 (ISO) and by MC according to the present paper. As exceptions, the primary estimate $y_0 = G(\mathbf{x})$

Table A1. Input data and results of the wipe test example.

Quantity	Symbol	Value	Standard uncertainty
Input data			
Gross effect			
Number of recorded events	n_g	2591	
Measurement duration	t_g	360 s	Neglected
Background effect			
Number of recorded events	n_0	41782	
Measurement duration	t_0	7200 s	Neglected
Wiped area	F, $u(F)$	100 cm^2	10 cm^2
Detection efficiency	κ, $u(\kappa)$	0.31	0.0155
Wiping efficiency	ε, $u(\varepsilon)$	0.34	$0.56/\sqrt{12}$
Lower and upper bounds of ε		0.06, 0.62	
Probabilities	α, β, γ	0.05	
Guideline value	y_r	0.5 Bq cm^{-2}	
Number of MC samples	N	10^6	
Quantity	Measurand: Y; Symbol	A_F (ISO) (Bq cm^{-2})	A_F (MC) (Bq cm^{-2})
Results			
Primary estimate	y_0	0.13227	0.13227
with standard uncertainty	$u(y_0)$	0.06604	0.06604
Best estimate	$\widehat{y}$	0.13590	0.1902
with standard uncertainty	$u(\widehat{y})$	0.06220	0.1452
Lower coverage interval limit	$y^<$	0.02170	0.0659
Upper coverage interval limit	$y^>$	0.26235	0.620
Decision threshold	y^*	0.02030	0.0323
Radiation effect present?	$y_0 > y^*$?	Yes	Yes
Detection limit	$y^\sharp$	0.11654	0.0953
Measurement procedure suitable?	$y^\sharp \leq y_r$?	Yes	Yes

and the associated standard uncertainty $u(y_0)$ follow from GUM and are thus identical in the ISO and MC cases. Only the significant digits of the MC results are indicated. These are the digits that barely changed in MC runs repeated several times with different independent histories. The MC-induced uncertainty of the MC results are $<2 \times 10^{-4}$ Bq cm^{-2} except $<1.3 \times 10^{-3}$ Bq cm^{-2} for the upper coverage interval limit.

The considerable differences between the corresponding results of the ISO and MC approaches are mainly due to the possibly small values of the wiping efficiency causing pronounced upper tails of distributions. This problem (b) should provide an incentive to revise the measurement procedure. Possibly, the wiping efficiency can be increased or the associated standard uncertainty reduced by using a more effective wiping material.

The wipe test example was especially designed to illustrate the problems that may occur in MC application. Moreover, the large differences between the corresponding ISO and MC results can make it clear that there are cases where an MC approach will be necessary and advantageous.

APPENDIX 4: MORE ABOUT MC-INDUCED UNCERTAINTY

In order to get a deeper insight into the matter of MC-induced uncertainty u_{MC}, the section dealing with this subject is here continued.

Consider a quantity $Z = g(\mathbf{X})$ that depends on ν other quantities X_i. Let estimates x_i of the latter quantities and the associated standard uncertainties $u(x_i)$ be known and the correlation coefficients be denoted by $r(x_i,x_k)$. If the function g is assumed to be sufficiently linear in a neighbourhood of $\mathbf{X} = \mathbf{x}$ determined by the known uncertainties, then, at least approximately, the estimate $z = g(\mathbf{x})$ of Z is associated with the standard uncertainty $u(z)$ given by[1,14,15]

$$u^2(z) = \sum_{i,k=1}^{\nu} \frac{\partial g}{\partial x_i}\frac{\partial g}{\partial x_k}\, u(x_i)u(x_k)r(x_i,x_k) \qquad \text{(A.42)}$$

where $\partial g/\partial x_i = \partial g/\partial X_i\,|_{\mathbf{X}=\mathbf{x}}$. Since $r(x_i,x_i) = 1$ and $|\,r(x_i,x_k)\,| \le 1$, equation (A.42) leads to an upper bound of $u(z)$ by applying $|\,a+b+\cdots\,| \le |\,a\,| + |\,b\,| + \cdots$ for arbitrary a, b, ... and then performing a square root:

$$u(z) \le \sum_{i=1}^{\nu} |\,\frac{\partial g}{\partial x_i}\,|\; u(x_i). \qquad \text{(A.43)}$$

Equality holds if $\nu = 1$. If, in particular, $Z = X_1/X_2$ with $x_1,\ x_2 > 0$, then $z = x_1/x_2$ and $\partial g/\partial x_1 = 1/x_2$ and $\partial g/\partial x_2 = -x_1/x_2^2$. This yields the relation

$$\frac{u(z)}{z} \le \frac{u(x_1)}{x_1} + \frac{u(x_2)}{x_2}. \qquad \text{(A.44)}$$

The sum of the relative standard uncertainties of the numerator and the denumerator of a fraction is thus always an upper bound of the relative standard uncertainty of the fraction even if the numerator and the denumerator are correlated. If they are uncorrelated, then

$$\frac{u(z)}{z} = \sqrt{\left(\frac{u(x_1)}{x_1}\right)^2 + \left(\frac{u(x_2)}{x_2}\right)^2}. \qquad \text{(A.45)}$$

Let $Z = X_1 - X_2$ with two MC-determined estimates $x_1 = J$ and $x_2 = J'$ of the same integral I. Then

$$u^2_{\mathrm{MC}}(J - J') = u^2_{\mathrm{MC}}(J) + u^2_{\mathrm{MC}}(J') - 2u_{\mathrm{MC}}(J)u_{\mathrm{MC}}(J')r(J,J') \qquad \text{(A.46)}$$

according to equation (A.42). This MC-induced uncertainty becomes a minimum if a strong positive correlation is present, i.e. if $r(J,\ J') = +1$. It even nearly vanishes if, in addition, $J \approx J'$ and, thus, $u_{\mathrm{MC}}(J) \approx u_{\mathrm{MC}}(J')$. This is the reason why J and J' should always be calculated with the same history of standard random numbers if the difference $J - J'$ is to be determined as in equation (37).

Let M represent any one of the counted numbers $N(\ldots)$ needed, for instance, in equations (28)–(33). It follows from a binomial distribution since every one of N samples is either counted with a probability p or not. This distribution has the standard deviation $\sqrt{Np\,(1-p)}$, which is the MC-induced standard uncertainty $u_{\mathrm{MC}}(M)$ associated with M. If p is not given, it is estimated by M/N. Then,

$$u_{\mathrm{MC}}(M) = \sqrt{\frac{M\,(N-M)}{N}};$$

$$\frac{u_{\mathrm{MC}}(M)}{M} = \frac{u_{\mathrm{MC}}(M/N)}{M/N} = \sqrt{\frac{1}{M} - \frac{1}{N}}. \qquad \text{(A.47)}$$

Notice $\sqrt{p\,(1-p)} \le 1/2$ in general and $= 0.21794$ for $p = 0.05$ and 0.95.

As an example of the application of equation (A.47), the probability $p = F_Y(q)$ of a given quantile q of some random variable Y is to be calculated by MC with a relative standard uncertainty $u_{\mathrm{MC}}(p)/p < 0.01$. How many samples are needed? Let $M = N(y_k \le q)$. Replacing the estimate M/N of p by p itself yields $u_{\mathrm{MC}}(p)/p =$

$\sqrt{1/(pN)-1/N} < 0.01$ or $N > (1/p-1)\times 10^4$. For an expected $p \approx 0.01, N > \approx 10^6$ samples are thus required.

For another application, $\widehat{y}$ according to equation (35) is considered with $M = N(y_k \geq 0\,|\,\mathbf{a})$ and equations (A.44) and (A.47). Then,

$$\widehat{y} \approx \frac{J_1}{J_0} = \frac{\overline{yH}}{M/N}; \tag{A.48}$$

$$u_{\mathrm{MC}}^2(J_1) = u_{\mathrm{MC}}^2(\overline{yH}) = \frac{1}{N(N-1)}\sum_{k=1}^{N}\left(y_k H(y_k) - \overline{yH}\right)^2 = \frac{J_2 - J_1^2}{N}; \tag{A.49}$$

$$\frac{u_{\mathrm{MC}}(\widehat{y})}{\widehat{y}} \leq \frac{u_{\mathrm{MC}}(\overline{yH})}{\overline{yH}} + \frac{u_{\mathrm{MC}}(M/N)}{M/N} = \sqrt{\frac{J_2/J_1^2 - 1}{N}} + \sqrt{\frac{1}{M} - \frac{1}{N}} \sim \frac{1}{\sqrt{N}} \tag{A.50}$$

since $M \approx Np$. In equation (A.49), the well-known expression for the (type-A[(1)]) uncertainty of a mean is applied. $N-1$ (or $N-3$ in BS[(22)]) is replaced again by the very large N (see also the text below equation (24)). The MC run may be stopped if $u_{\mathrm{MC}}(\widehat{y})/\widehat{y}$ becomes sufficiently small.

The number N of samples and the MC-induced uncertainty can also be assessed by applying the uncertainty equation (A.43) with $\nu = 1$ to, for instance, the type-B integral according to equation (36), i.e. to $I(\eta) = \int_c^{\eta} f(x)\mathrm{d}x = \varepsilon \approx M/N$ with $M = N(c \leq x_k \leq \eta)$ and the constants c, ε and N. Equation (A.43) then reads $u_{\mathrm{MC}}(I) = |\,\mathrm{d}I/\mathrm{d}\eta\,| \times u_{\mathrm{MC}}(\eta) = f(\eta)u_{\mathrm{MC}}(\eta) \approx u_{\mathrm{MC}}(M)/N$. Inserting $u_{\mathrm{MC}}(M) = \sqrt{N\varepsilon(1-\varepsilon)}$ and solving for N finally leads with $f(\eta) \approx (J(\eta_1) - J(\eta_0))/(\eta_1 - \eta_0)$ to

$$N \approx \frac{\varepsilon(1-\varepsilon)}{f^2(\eta)u_{\mathrm{MC}}^2(\eta)};$$

$$u_{\mathrm{MC}}(\eta) \approx \sqrt{\frac{\varepsilon(1-\varepsilon)}{N}} \cdot \left|\,\frac{\eta_1 - \eta_0}{J(\eta_1) - J(\eta_0)}\,\right|. \tag{A.51}$$

The estimates $J(\eta_0)$ and $J(\eta_1)$ should again be determined by using the same history of standard random numbers. If a centred normal distribution $f(\eta) = \exp(-\eta^2/(2\sigma^2))/\sqrt{2\pi\sigma^2}$ and the ε-quantile $\eta = -1.65\sigma$ for $\varepsilon = 0.05$ with $c = -\infty$ is considered and, moreover, $u_{\mathrm{MC}}(\eta) = 0.01\sigma$ is required, then at least $N \approx 4.5 \times 10^4$ samples are needed. Numbers N of a similar order of magnitude, mainly determined by $1/u_{\mathrm{MC}}^2(\eta)$, are obtained with other distributions. Equation (A.51) can be applied to the integrals I_3, I_4, I_5 and I_7.

The MC-induced standard uncertainty $u_{\mathrm{MC}}(\eta)$ associated with the solution η of a type-C integral, namely the detection limit $\eta = y^{\sharp}$, can be obtained similarly to equation (A.51). But the standard uncertainty $u_{\mathrm{MC}}(b)$ associated with the already MC-determined upper integral limit $b = y^*$, the decision limit, must in addition be taken into account. Let $I = I(\eta,b)$, then $\mathrm{d}I = (\partial I/\partial\eta)\mathrm{d}\eta + (\partial I/\partial b)\mathrm{d}b$ or

$$\frac{\partial I}{\partial \eta}\mathrm{d}\eta = \mathrm{d}I - \frac{\partial I}{\partial b}\mathrm{d}b;$$

$$\frac{\partial I}{\partial b} \approx A = \frac{J(b_1,\eta) - J(b_0,\eta)}{b_1 - b_0};$$

$$\frac{\partial I}{\partial \eta} \approx B = \frac{J(b,\eta_1) - J(b,\eta_0)}{\eta_1 - \eta_0} \tag{A.52}$$

and, accordingly, with $(\mathrm{d}z)^2$ replaced by $u_{\mathrm{MC}}^2(z)$ for any quantity z and if b and η are determined by using independent histories to avoid a correlation,

$$\left(\frac{\partial I}{\partial \eta}\right)^2 u_{\mathrm{MC}}^2(\eta) = u_{\mathrm{MC}}^2(I) + \left(\frac{\partial I}{\partial b}\right)^2 u_{\mathrm{MC}}^2(b). \tag{A.53}$$

With $u_{\mathrm{MC}}^2(I) = \varepsilon(1-\varepsilon)/N$ as derived in the preceding paragraph, this finally yields

$$u_{\mathrm{MC}}^2(\eta) \approx \frac{\varepsilon(1-\varepsilon)/N + A^2 u_{\mathrm{MC}}^2(b)}{B^2} \tag{A.54}$$

This equation can be applied to I_6 for $\eta = y^{\sharp}$ and $b = y^*$. Then, $u_{\mathrm{MC}}^2(y^*)$ to be inserted can be obtained from equation (A.51) by using an independent history.

APPENDIX 5: GLOSSARY OF SOME IMPORTANT TERMS AND SYMBOLS

Z	general random variable, general estimator of a physical quantity
z, ζ	values of Z
Y	estimator assigned to the measurand; also used for the measurand itself

y	value of Y, general estimate of the true measurand value, possible true measurand value if $y \geq 0$; particular values y are marked by affixes
$u(y)$	measurement uncertainty of Y associated with y; standard uncertainty if y is the expectation of Y
$\mathbf{a}$	information set of data, conditions, assumptions, relations and other relevant information
$f_Y(y \mid \mathbf{a})$	distribution (probability density) of Y on the information $\mathbf{a}$
$F_Y(y \mid \mathbf{a})$ $= \Pr(Y \leq y \mid \mathbf{a})$ $= \int_{-\infty}^{y} f_Y(\eta \mid \mathbf{a}) \mathrm{d}\eta$	distribution function of Y on the information $\mathbf{a}$
$\mathbf{X}$	vector of input quantity estimators X_i
$\boldsymbol{\xi}$	vector of general values ξ_i of X_i
$f_{\mathbf{X}}(\boldsymbol{\xi} \mid \mathbf{a})$	distribution of $\mathbf{X}$ on the information $\mathbf{a}$
$G(\mathbf{X})$	model function, $Y = G(\mathbf{X})$ model equation
$\mathbf{x}$	vector of given particular values of $\mathbf{X}$
$\widetilde{y}$	assumed true measurand value
$\widetilde{\mathbf{a}}(\widetilde{y})$	modification of $\mathbf{a}$ as a function of $\widetilde{y}$
y_0	primary estimate of the true measurand value
$\widehat{y}$	best estimate of the true measurand value
$y^{\triangleleft}, y^{\triangleright}$	lower and upper limits of the coverage interval
y^*	decision threshold
$y^\sharp$	detection limit
y_k	MC samples ($k = 1, \ldots, N$)
$y^{(k)}$	MC samples y_k sorted by magnitude and renumbered
N	total number of MC samples y_k
$N(\text{conditions} \mid \text{parameters})$	number of MC samples y_k meeting the conditions
u_{MC}	MC-induced standard uncertainty
α	probability of the physical effect being falsely recognised as present, although $\widetilde{y} = 0$ (error of the first kind)
β	probability of the physical effect being falsely recognised as absent, although $\widetilde{y} > 0$ (error of the second kind)
$1 - \gamma$	coverage probability; probability that the coverage interval contains the true measurand value
I, J	a particular integral and its estimate
t	duration of measurement