CALCULATION OF DETECTION LIMITS BY EXPLICIT EXPRESSIONS

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ABSTRACT

A method for calculating an approximate value of the detection limit for measurements of ionizing radiation is presented. The method can be applied when the uncertainty of the indication, corresponding to the detection limit, is given as an explicit function of the indication. Then also the detection limit can be calculated explicitly, which means that the iteration procedure for its calculation can be avoided. The advantage of the method becomes apparent when the iteration process for calculating the detection limit is difficult to apply.

INTRODUCTION

According to the standard ISO 11929 (ISO 2010) the decision threshold and the detection limit are expressed in terms of the value of the measurand and its uncertainty. Whereas the decision threshold is expressed by the uncertainty of the measured value if the conventional value of the measurand is zero, the detection limit is calculated from the uncertainty of the measurand having the value of the detection limit, i.e., the value of the measurand that can be recognized with a predefined probability. It is easy to see that from this method of calculation an implicit equation follows, that in general cannot be solved in a closed form, but by iteration only.

Two sources of uncertainty contribute to the uncertainty of the measurand: the uncertainty of the indication and the uncertainty of the conversion factor, which converts the indication into the value of the measurand. However, in the methods of calculation of the decision threshold and the detection limit the two uncertainties do not play equivalent roles; therefore, by separating both sources of uncertainty and treating them differently, expressions can be derived that can be used for calculating the detection limit instead of the iteration process. The calculation can be divided into two steps: in the first step the indication corresponding to the detection limit is calculated and in the second the detection limit itself is calculated. To do this, from the uncertainty of the indication as a function of its value, approximate expressions can be derived that make it possible to express the detection limit in an explicit, although approximate, form. The method is validated by applying it to two cases where the detection limit can be expressed in an exact explicit form by comparing the approximate results with the results obtained from exact expressions: for the case when the uncertainty of the indication does not depend on its value and for the case elaborated by Currie (Currie, 1968).

METHODS

The standard ISO 11929 defines the detection limit as

$$y^{\#} = k_{1-\alpha} \cdot u(0) + k_{1-\beta} \cdot u(y^{\#}) \qquad (1)$$

where $y^{\#}$ denotes the detection limit, $u(0)$ is the null measurement uncertainty, $u(y^{\#})$ is the uncertainty of the measurand at the detection limit and $k_{1-\alpha}$ and $k_{1-\beta}$ are the quantiles of the standardized normal distribution corresponding to the predefined probabilities α and β for making errors of type-I and type-II respectively.

In radiation measurements the measuring function is (ISO 2010)

$$y = w \cdot n_n \qquad (2)$$

where n_n is the net indication, i.e., the part of the indication originating in the measurand, and w denotes the conversion factor converting the net indication into the observed value of the measurand. Therefore a relation among the indications, equivalent to Eq. (1) follows

$$n_n^{\#} = k_{1-\alpha} \cdot u(n_n=0) + k_{1-\beta'} \cdot u(n_n^{\#}) \qquad (3)$$

where $n_n^{\#}$ and $u(n_n=0)$ are the indications corresponding to the detection limit and the null measurement uncertainty of the indication, respectively. It is easy to see that $k_{1-\beta'}$ is given by

$$k_{1-\beta'}^2 = k_{1-\beta}^2 \cdot [1 + u_{rel}(w)^2 \cdot n_n^{\#2} / u(n_n^{\#})^2] \ , \qquad (4)$$

where $u_{rel}(w)$ denotes the relative uncertainty of w. This quantile corresponds to the probability β' of the indication, which takes into account the uncertainty of the conversion factor and in Eq. (3) replaces the quantile corresponding to the predefined probability β. It is clear that Eq. (4) presents an implicit equation for $k_{1-\beta'}$, since the relative uncertainty $u(n_n^{\#})/n_n^{\#}$ depends on it. Consequently, the application of Eq. (4) and the expression for $u(n_n^{\#})$ as a function of $n^{\#}$ represents an approximative method for calculating the detection limit of the indication, as an alternative to the method using iteration.

EXAMPLES

The simplest case for applying the method occurs when $k_{1-\alpha} = k_{1-\beta}$ and the uncertainty of the background indication dominates the uncertainty budget of the net indication, therefore $u(n_n^{\#}) = u(n_n=0)$. Then the detection limit assumes the well-known expression

$$y^{\#} = \frac{2\, y^*}{1 - k_{1-b}^2 \cdot u_{rel}^2(w)} \qquad (5)$$

To illustrate the method on a more complex example, the case considered by Currie (Currie, 1968), where the uncertainty of the indication given by

$$u(n_n^{\#})^2 = u(n_n = 0)^2 + n_n^{\#} \qquad (6)$$

is presented. For this case the exact solution for the detection limit exists, therefore the detection limits calculated by solving the Eq. (4) and calculating $n_n^{\#}$ can be compared with exact values. In the comparison it is supposed that the background is 10^2 counts and that the factor converting the net counts registered during the acquisition time to the measurand is $w = 10^{-2}$ s^{-1}. The decision threshold is calculated for a probability of 1 % for making type-I errors i.e., $k_{1-\alpha} = 3.47$. The detection limit is calculated supposing a probability of 5 % for making errors of type-II, i.e., $k_{1-\beta} = 1.65$. The uncertainty of the background is $u(n_B) = 10$; therefore, the null measurement uncertainty is $u(0) = 0.14$. A relatively small number of background counts and a large difference in $k_{1-\alpha}$ and $k_{1-\beta}$ are used in the example in order to increase the influence of the net indication and the difference of the quantiles on the detection limit. The comparison is presented on Table 1.

Table 1: The exact values of the detection limits, the values of the quantile $k_{1-\beta'}$ and the approximate values of the detection limit, obtained from Eq. (4) followed by calculating $n_n^{\#}$

$u(w)/w$	$y^{\#}$, exact / s^{-1}	$k_{1-\beta'}$	$y^{\#}$, by Eq. (4) / s^{-1}
0.02	0.765	1.651	0.765
0.05	0.772	1.686	0.772
0.10	0.795	1.810	0.795
0.20	0.898	2.349	0.896
0.40	1.569	6.132	1.630

CONCLUSIONS

The application of the approximate method is advantageous in cases when the exact expression for the detection limit is not known or the iteration is difficult to apply. This occurs when $u(n_n=0)$ is obtained e. g. with the method of least squares by fitting a spectral region. Then, in successive approximations the uncertainties $u(n_n^{\#}{}_i)$ are obtained by the method of least squares as well. To perform the calculation, the number of counts in the i-th step of the iteration corresponding to the detection limit, $n_n^{\#}{}_i$, representing the response of the detection system to the measured quantity having the value corresponding to the detection limit, has to be inserted into the spectral region. Since the uncertainty of the $n_n^{\#}{}_i$ counts depends on the spectral shape, additional suppositions have to be used in order to define how the additional $n_n^{\#}{}_i$ counts are distributed over the spectral region.

REFERENCES

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