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Calculation of the decision thresholds for radionuclides identified in gamma-ray spectra by post-processing peak analysis results

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ABSTRACT

A method for calculating the decision thresholds for gamma-ray emitters, identified in gamma-ray spectrometric analyses, is described. The method is suitable for application in computerized spectra-analyzing procedures. In the calculation, the number of counts and the uncertainty in the number of counts for the peaks associated with the emitter are used. The method makes possible to calculate decision thresholds from peaks on a curved background and overlapping peaks. The uncertainty in the number of counts used in the calculation was computed using Canberra's Standard Peak Search Program (Canberra, 1986, Peak Search Algorithm Manual 07-0064). For isolated peaks, the decision threshold exceeds the value calculated from the channel contents in an energy region that is 2.5 FWHM wide, covering the background in the immediate vicinity of the peak. The decision thresholds vary by approximately 20% over a dynamic range of peak areas of about 1000. In the case of overlapping peaks, the decision threshold increases considerably. For multi-gamma-ray emitters, a common decision threshold is calculated from the decision thresholds obtained from individual gamma-ray emissions, being smaller than the smallest of the individual decision thresholds.

1. Introduction

The standard ISO 11929 [1] requires documenting of the decision threshold, regardless of whether the radionucleus of interest was identified in the gamma-ray spectrum or not. Also, the standard ISO 18589-3 [2] recommends reporting of decision thresholds as supplementary information irrespectively on the identification of the gamma-ray emitter. However, the conditions in which the decision threshold is calculated differ significantly when the gamma-ray emitter is not identified in the spectrum from the conditions when it is. In the first case the measurement presents a null measurement, i.e. a measurement where the specified measured quantity value is zero; therefore, here for the calculation of the decision threshold the measured spectrum is used. When the gamma-ray emitter is identified, the null measurement may not exist; therefore, the information from the measured spectrum has to be modified as to approximate the conditions being encountered in the null measurement.

Usually, in gamma-ray spectrometry, the calculation of the decision thresholds and the detection limits is the last step in the spectrum analysis. At that stage, the results of the data reduction from the channel contents to the peak properties, i.e., the peak positions, areas and widths, are already known. In this case the indications provided by the spectrometer are the peak areas. It is also known which gamma-ray emitters are present in the sample and their activities, provided that the peak location was performed at a sensitivity that allows for the detection of peaks with an area smaller than the number of counts corresponding to the decision threshold. Then it can be supposed that the radionuclides present in the sample at an activity exceeding the decision threshold are recognized with a large probability. It follows that for the identified radionuclides, the specified quantity value (the activity or the activity concentration) is larger than zero, and for the unidentified radionuclides, the specified quantity value is zero.

Whereas for gamma-ray emitters that are detected in the sample, the data that are needed for the calculation of the characteristic limits are accessible from the results of the peak analysis; for gamma-ray emitters not detected, these data are not available. Therefore, to calculate the decision threshold and the detection limit for unidentified radionuclides, the raw spectral data, i.e., the channel contents, must be used [3,4], whereas the calculation of the decision thresholds and the detection limits for the identified radionuclides can be based on the results of the peak analysis. Calculating decision thresholds from peak-analysis results simplifies the calculation considerably, because the data on the peaks, and the conversion factors, converting the counts into activities or activity concentrations, are already calculated during the peak analysis and the activity calculations.

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It is the purpose of this paper to present a method for calculating the decision threshold from the results of the peak analysis and the results of the activity calculation.

2. Methods

In gamma-ray spectrometry the activities or activity concentrations are calculated using the measurement model

$$y = n_n w \tag{1}$$

where n_n denotes the net indication, i.e., the number of counts in a peak, belonging to the measurand, and w denotes the conversion factor, needed to convert the number of counts into the activity or activity concentration.

The net indication may not correspond to the whole area of a peak, because a bias may be present, originating in the spectrometer background, the presence of interfering nuclei in the sample or the contribution of a blank sample. Therefore, the net indication, n_n, is given by the total number of counts in the peak n_p, as

$$n_n = n_p - n_B \tag{2}$$

where n_B denotes the number of counts in the peaked background, representing the bias.

In computerized gamma-ray spectrometry analyses the peak areas are calculated using the peak-analyzing software. The peak-analysis algorithms calculate the peak area supposing a width of the peak region, which is not related directly with the FWHM of the peak retrieved from the FWHM calibration of the spectrometer. Also, they report the number of counts in the continuous background only, disregarding the possible contributions of the neighboring peaks [5]. To arrive at the number of counts in a peak region, which do not belong to the peak, it is therefore necessary to define the width of the peak region basing on the FWHM from the calibration. Then the peak region comprises a predefined fraction of the number of counts in the peak and the total number of counts is related with the number of counts in the peak and the number of counts, which do not belong to the peak as follows (Fig. 1):

$$n_g = n_0 + n_p \tag{3}$$

where n_g denotes the total number of counts in the peak region and n_0 the number of counts that do not belong to the peak. For isolated peaks the number of counts in the peak region, which do not belong to the peak, equals to the number of counts in the continuous background. For overlapping peaks besides the continuous background also counts belonging to the neighboring peaks contribute.

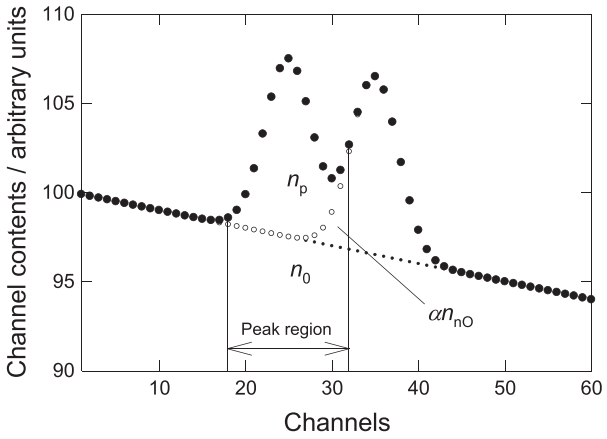

Fig. 1. Schematical presentation of a peak region. n_p denotes the number of counts in the peak, n_0 the number of counts in the total background within the peak region and αn_{nO} the counts belonging to the overlapping peak which are registered within the peak region.

For calculating the decision threshold, y^*, the uncertainty of the blank indication $u_B(n_n=0)$ is needed; this depends on the uncertainty of the bias and the uncertainty in the number of counts in the peak region that do not belong to the net indication. Since the bias is determined from separate measurements, i.e., background measurements and the measurements of blank samples, or peak areas belonging to the possible interfering gamma-ray emitters, the number of counts in the continuous background is statistically independent of the number of counts in the peaked background. Therefore, the uncertainty in the blank indication can be calculated as

$$u_B^2(n_n = 0) = u^2(n_n = 0) + u^2(n_B) \tag{4}$$

where $u(n_n=0)$ denotes the uncertainty in the blank indication at a vanishing uncertainty of the bias $u(n_B)$. While the peaked background and its uncertainty are retrieved from sources that are independent of the peak, the number of counts in the peak region that do not belong to the peak, with its uncertainty, must be calculated from the total number of counts in the peak region and the peak area and its uncertainty, which are reported by the peak-analysis software [6].

By Eq. (3) the counts in the peak region are divided between the counts belonging to the peak and the counts, which do not belong to the peak. Because n_p and n_0 refer to the same total number of counts n_g, they are correlated with the correlation coefficient -1, expressing the requirement that counts, which belong to the peak, do not belong to the background where it resides. Supposing that the width of the peak region is fixed, the standard deviation of the total number of counts is given by the Poisson statistics. The standard deviation of the number of counts in the peak, $u(n_p)$, is reported by the peak analyzing software, therefore the uncertainty of the number of counts, which do not belong to the peak, $u(n_0)$, is given by [7], taking into account the correlations among n_g, n_p and n_0

$$u^2(n_g) = u^2(n_p) + u^2(n_0) - 2u(n_p)u(n_0) \tag{5}$$

where $u(n_g)$ denotes the uncertainty of the total number of counts in the peak region. This equation has two solutions

$$u(n_g) = \pm\left[u(n_p) - u(n_0)\right] \tag{6}$$

and since $u^2(n_g) = n_g$, the uncertainty in the number of counts in the background under the peak can be calculated as

$$u(n_0) = u(n_p) \pm \sqrt{n_g}. \tag{7}$$

When calculating $u(n_p)$, the peak analyzing software takes into account the uncertainties of channel contents in the peak region which are given by the Poisson distribution and the uncertainty of the number of counts in the background under the peak. The information on the number of background counts must at least partially originate in channel contents outside the peak region, therefore $u(n_p)$ must exceed $n_g^{1/2}$. Because the difference is always positive, it follows that both values for $u(n_0)$ in Eq. (7) describe possible cases encountered in peak analysis. Both solutions quantify circumstances, which may be encountered in the spectrum analysis. In Annex I it is shown that the smaller value describes the uncertainty of the background under isolated peaks, whereas the larger value describes the uncertainty of the background in case of overlapping peaks.

In the derivation of the decision threshold it is assumed that neither the continuous background nor the areas of neighboring peaks depend on the area of the peak corresponding to the energy where the decision threshold is calculated. Therefore it is assumed that also $u(n_0)$ describes the uncertainty of the background under the peak in measurements of blank samples. For the calculation of