VERIFICATION OF GAMMA-SPECTROSCOPY PROGRAMS:
ACCURACY
AND DETECTABILITY

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The newly revised ANSI N42.141~2 has provided analysis software developers with a set of well defined, consistent and unbiased procedures designed to evaluate the accuracy and limitations of peak search and peak area analysis programs. This work uses two of the procedures outlined in this standard to evaluate five peak analysis algorithms currently in use in Canberra and Nuclear Data software packages. The first procedure examines a program's behavior as the centroid separation and peak height ratio of a doublet are varied. A previous review of these data3 demonstrated significant peak area inaccuracies at peak separations at or below 1.5 FWHM. We will discuss improvements made to some of these programs and the impact on the doublet results. The second procedure examines a program's behavior as the Compton continuum beneath a fixed peak area is increased. For the same five algorithms we will discuss the dependence of peak area on Compton continuum and also explore the limits of peak detectability.

Introduction

As automated gamma-ray data acquisition and analysis systems have become more commonplace, and indeed are being used in production rather than research environments, the need for a simple yet sensitive verification scheme has become more acute. The newly released revision to ANSI N42.141~2 details in a very straightforward fashion the steps an operator of a germanium detector based gamma-ray spectrometer can use to verify the performance of the system. Here the "system" is defined not only to be the detector, front-end pulse shaping electronics and multi-channel analyzer but also the computer and data reduction software used to analyze the spectral data. The standard is designed to be used by laboratory personnel who have some, but not extensive, experience in gamma-ray spectroscopy.

The standard is also useful for commercial software developers as a verification tool. The basic procedures in the standard can be easily extended and generalized to allow for more systematic studies of software performance. In this paper we will use two of the software verification procedures proposed in the ANSI standard. The first procedure tests the ability of the software to accurately quantify the net areas of two closely lying photo-peaks as the separation and relative peak heights are varied. A previous investigation of these data3, as applied to existing Canberra and Nuclear Data (ND) software, uncovered some problems in net area accuracy at peak separations at or below 1.5 FWHM. This is primarily a problem for software which allows for manual addition of peaks, as most peak locate algorithms cannot separate peaks that are less than 1.5 FWHM apart. New results for SAMPO 90 and the ND standard peak search based on improved algorithms are presented in this study.

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The second procedure in the ANSI standard tests the ability of software to find and properly quantify single peaks as the Compton continuum underneath the peak is increased. As data were analyzed a quality factor $k$, reflecting the peak-to-background ratio, was associated with each peak area. To do this in a statistically significant fashion the critical level concept, as introduced by Currie, was used. Even though the critical level, as well as detection limits, were derived assuming gross counters, these same concepts are applicable to gamma-ray spectroscopy as well.

Many software packages, including some Canberra and Nuclear Data packages, use the critical level as a decision level. Typically a peak search function uses a finite difference method to find potential peak regions. After region limits are established net peak areas are computed by subtracting an estimate of the Compton background. The critical level is given by the equation:

$$\text{CriticalLevel} = K \sqrt{b + \sigma_b^2}$$

where $b$ is the Compton background, $\sigma_b$ is the standard deviation in $b$ and $K$ is a statistical factor which defines the false positive rate (saying that a peak is present when it actually is not) you are willing to tolerate. Since many programs do not provide an estimate of $\sigma_b$, a common simplifying assumption is that the background follows Poisson counting statistics, which implies

$$\text{CriticalLevel} = K \sqrt{2 \cdot b}$$

While technically incorrect, this assumption allowed for a consistent definition of our peak quality factor from package to package. In most applications, the 95% confidence level is chosen; which means $K = 1.645$. In some software packages, if the net peak area exceeds the critical level it is deemed to be a "true" peak; if not the peak region is discarded.

In this study, we define a peak quality factor $k$ as shown below since it is directly related to the statistical factor $K$ in the critical level equation.

$$k = \frac{A}{\sqrt{2b}}$$

where $A$ is the net peak area. We will investigate the behavior of the peak detection and quantification algorithms as $k$ decreases to values at or near 1.645, in other words as peak areas approach the critical level.

Experimental Methods

The test spectra used for this investigation were acquired with a standard high-purity germanium detector in a coaxial geometry. This detector has a relative efficiency of 16.5% and a resolution of 1.75 keV at 1332 keV. The pulse shaping electronics consisted of a Canberra Model 2020 spectroscopy amplifier with a 4 microsecond shaping time, a Model 579 Wilkinson-type ADC with a conversion gain of 4096 channels, and a Model 556 Ethernet Acquisition Interface Module (AIM). The amplifier gain was adjusted to obtain a 0.5 keV/channel energy calibration.