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Choice of computer software for analysis of spectra from the Multi-spectral Logging System

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Abstract

We have investigated the range of software available for determination of elemental concentration from gamma-ray spectra, to learn which are most suitable for use with the Multi-spectral Logging System being developed for the Department of Energy. We believe that the spectrum fitting method will be more satisfactory than the peak-matching method.

Introduction

The successful completion of the field tests of the prototype Multi-spectral Logging System (MLS) (Conaway and Frankle, 1994) emphasizes the need for software that can be used to automatically compute elemental concentrations from the spectra obtained from the system. The detection threshold for an element depends not only on the hardware used to obtain the spectrum, but also on the software used to analyze the data. If the software is not optimal, many of the benefits of improved hardware are lost.

The nuclear spectroscopy industry has spent decades developing software for spectral analysis. Available systems are user-friendly, fast, automatic, and work well on modern personal computers. They are, however, designed for spectra obtained from activation of small samples for long times under ideal conditions. These spectra consist of sharp, Gaussian peaks superimposed on a minimal background.

When spectra are obtained in the field, using a neutron generator and recording gamma rays from not only activation but also prompt capture, and with the short counting times needed for a practical logging tool, the shapes of the peaks are quite different. The figure shows part of two spectra (on the same energy scale) from the MLS, one from an 8-hour count in the laboratory on a reactor-activated sample (the type of spectrum for which conventional software is designed) compared to one from a 100-sec count from a sample activated by the neutron generator in a borehole.

Part of the difference in the spectrum is due to statistics: The Poisson distribution from the short counting time degrades the quality of the data. But more important is the sample shape. The reactor sample is small, and close to the detector. Most gamma rays reach the detector without scattering. On the other hand, in the borehole many of the gammas that reach the detector have travelled through many centimeters of the formation, and have been scattered in the process. Therefore only a fraction of the detected gammas have the full energy typical of the peaks; the others contribute to the background. No improvement in hardware or increase in counting time can cope with this situation; the scattering occurs before the gammas reach the detector.

Moreover, spectra obtained from a combination of capture and activation a few tens of μ s after a neutron pulse contain many more peaks than spectra obtained by activating a sample by some convenient method, waiting some time, and then placing the sample near a detector. This situation is an advantage in that the more peaks that can be used to identify a nuclide the more positive the identification, but it is a disadvantage in that the software must cope with this multiplicity of peaks.

The purpose of this report, therefore, is to investigate the range of software available for determination of elemental concentration from gamma-ray spectra, and attempt to recommend which is the most satisfactory for the MLS.

There are two fundamentally different types of programs available for the task. Most systems analyze the spectrum peak by peak, and use the amplitudes of one or more peaks to determine the concentration of the nuclide giving rise to the peak. These we shall call "peak-matching" programs. A

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few systems use the entire spectrum from each element, and make a least-squares fit of the amplitudes of the spectra to obtain the concentration of the element giving rise to the spectrum. These we shall call "spectrum-fitting" programs. We shall treat each in turn

It should be noted that at least two studies (University of Costa Rica, 1991; Decker and Sanderson, 1992) comparing several peak-matching programs have been published. Unfortunately, they are not applicable to the problems of the MLS.

The peak-matching method: principles

The first step in a peak-matching program is the definition of peak shape. Some programs use a Gaussian shape, some permit user-defined shapes, and some do not specify shape. Often the peak is located by a least-squares fit to the defined shape. The next step is calculation of background for each peak. The sophistication of the background calculation depends on the sophistication of peak shape definition. Once the background has been calculated for each peak, the area, centroid, and FWHM can be calculated for each, again using fits to the defined shape.

The next step is calibration (or recalibration.) Generally a few known peaks are used to fit a curve of peak energy vs channel number. The curve is not necessarily linear; frequently it is taken to be a polynomial. The efficiency is calibrated using the areas of peaks from sources with known activity. Some programs use additional procedures to redefine the peak shape using data from calibrated peaks.

After the system has been calibrated, and all the peaks located, the peak energies are compared to the energies of peaks in a library of known peaks from nuclides expected to be seen. Often peaks overlap, and some method must be used to deconvolve multiplet peaks. Once all peaks are identified (or perhaps many peaks are identified, and some cannot be identified and are ignored) a procedure is used to convert the areas of the identified peaks to the concentration (or "activity") of the nuclide to which the peak is attributed. The list of abundances is the output of interest.

It appears that although the available programs use different methods of peak identification and calibration, all are well described in the literature, and there is no need to describe them here. All are quite adequate for conventional spectral analysis. The methods of calculating concentration, however, are quite different, and their potential applicability to the MLS is correspondingly different. Therefore they should be discussed individually. This study is based on the published algorithms for each of three commercial programs and a description of a DOE program.

The peak-matching method: software available for calculating elemental concentration

OSQ/Plus by APTEC Nuclear

This program (APTEC, 1991), fits Gaussian shapes to peaks. It calculates the concentration (activity) from a given photopeak using the area under that peak with appropriate corrections for branching ratio, decay (assuming a known decay constant and time between sample collection and spectral acquisition), and sample volume. Multiplets are deconvolved using a digital filter. There is no procedure for using more than one peak simultaneously to estimate concentration.

FITEK by W. Stoeffl

This program, which is undocumented and runs only on a VAX is said (Dougan, 1994) to be extremely versatile and particularly useful for comparing several spectra at once. Since it is undocumented, we are unable to describe it.

Genie-PC by Canberra Nuclear

This program (Canberra, no date) uses a modified Gaussian as a description of the peaks. The user supplies peaks whose shape is assumed to be that of all peaks to be analyzed, and the program

computes a "tail parameter" to add to the conventional Gaussian form. Multiplets are deconvolved with a non-linear least squares procedure. The nuclide identification procedure uses a matrix formalism similar to that developed in SAMPO80 (Koselko et al., 1981), which is based on the ideas originally presented by Gunnink (Gunnink and Niday, 1972.) All nuclides that pass a set of acceptance criteria are included in a matrix with one column for each identified nuclide and one row for each identified peak. The entries in the matrix elements are the appropriate gamma branching probabilities for each nuclide and peak. If there are no interferences (i.e., a given nuclide has no peak in common with any other nuclide) then the concentration represented by each peak is calculated from the area under the peak with appropriate corrections for branching ratio, decay, and sample volume. Then the final value of concentration is determined by weighted averaging of the concentrations obtained from each peak. If interferences between nuclides are present, the portion of the matrix represented by those nuclides is solved for the fraction of each peak due to each nuclide, and that fraction used as the area in the concentration calculation.

Gamma-Vision by EG&G Ortec

This program (Ortec, no date) describes peaks as pure Gaussians. Multiplets are deconvolved using a matrix procedure that is not described in detail. Concentration is determined from peak areas with a correction for branching ratio. Decay correction is optional. The final value of concentration is determined by weighted averaging of the concentrations obtained from each peak.

GAMMAW by W. Westmeier

This program (Westmeier, no date) describes peaks as modified Gaussians, with an expression for the low-energy tail developed by the author. Concentration is determined by a weighted average of concentrations obtained from individual peaks. The author is willing to adapt it to specific situations.

LGALC by R. Price of Westinghouse Hanford Company

This program (Stromswold, 1994) is designed specifically for borehole logging, but only for passive gamma-ray logging, not for prompt capture gamma-rays. The method of peak location and area calculation is much simpler than those used in commercial software; no peak shape is assumed. It has no procedure for dealing with multiplets, and the program can deal with only a few peaks. Concentration is determined from peak areas corrected for detector efficiency, steel casing in the borehole, water in the borehole, and shielding in the logging sonde. The use of weighted averaging of data from multiple peaks is being considered as an improvement.

The spectrum fitting method

Spectrum-fitting programs for well-logging applications were first developed for use with NaI detectors (Hertzog, 1980.) Standard spectra of neutron-induced and natural gamma rays are obtained for each element that is expected to be encountered in the formation. These spectra are produced in models whose geometry approximates realistic field geometry. Consequently the effects of attenuation of the gamma-rays by the formation is included in the standard spectrum. A spectrum of gamma-rays created in the logging sonde itself is also produced. Then the field spectrum is analyzed by assuming it to be a linear combination of standard spectra, and a least-squares fit is made to obtain concentrations of the elements represented by the standard spectra. This procedure has been a very successful, and is in use worldwide. It is, however, limited to a specific set of elements for which standard spectra can be readily obtained, and detection thresholds are higher than those required for environmental problems envisioned in the design of the MLS (Kerr et al., 1992.)

A spectrum-fitting procedure for germanium spectra from neutron-induced gamma-rays has been proposed for borehole use (Jin et al., 1987) and developed for analysis of coal samples on a conveyor belt (Shyu et al., 1993.) Standard spectra were developed by Monte Carlo modeling of realistic geometries and logging sondes rather than measurement using physical models. Physical models were used to benchmark the Monte Carlo models. In this way it is feasible to obtain detailed spectra for elements having low

concentration in a matrix of other materials. Unfortunately, that work has been abandoned, and no software is available at present.

Another similar procedure for spectra from thick assemblies of actinides has been developed in an effort to improve nuclear weapons safeguards (Gosnell, 1990; Gosnell and Pohl, 1994.) No neutron irradiation is involved, but the complex actinide standard spectra, simulated by Monte Carlo calculations, are similar to those that would be obtained by a logging system. A proposal has been made to calculate standard spectra for logging problems, but no work has been done as yet.

Recommendations

The only reliable way to determine whether a program is suitable for analysis of a given type of spectrum is to obtain typical samples of that type of spectrum and observe how well the program performs. In the absence of good sample spectra, it is necessary to draw conclusions from descriptions of the programs.

In principle, one could adapt a peak-matching program for borehole use by modifying the peak shape to account for the attenuation of gamma-rays in the formation, and applying corrections similar to those in *LGALC*. Many gammas, however, are scattered entirely out of the peak and considered part of the background. In the spectrum-fitting method, on the other hand, all of the gammas from the elements of interest are still present in the spectrum, albeit in what appears to be the continuum. Consequently it has been estimated that the detection threshold for a given element could be as much as an order of magnitude lower using the spectral-fitting method rather than the peak-matching method simply because of better statistics.

Another difficulty in modifying a peak-matching program is the fact that all of the useful programs are proprietary, and it is unlikely that the source code would be available. The germanium-spectral-fitting programs, on the other hand, have been developed by a university and a national laboratory, both of which organizations would probably be happy to cooperate in modifications.

In the short term, a peak-matching program must be used, because at present no spectral-fitting program is available for routine use. The most plausible candidate appears to *Genie-PC*, because it has two characteristics which seem to make it appropriate for dealing with MLS problems. First, it permits some modification of peak shapes, with the user controlling the modification. This makes it possible to adapt the program to peak shapes encountered in MLS spectra. Second, because it uses a sophisticated matrix procedure for determining elemental concentrations, rather than averaging the concentrations determined from individual peaks, it seems to be the most capable of the peak-matching programs for dealing with the complex, poor-quality spectra arising from the MLS.

In the long term, the spectral-fitting procedure should be adapted to the MLS. This type of program is inherently capable of dealing with the spectra to be expected. The major task will be the development of a large library of standard spectra. This can be accomplished with Monte Carlo calculations and a minimum number of benchmark experiments.

It seems quite possible that with an optimized analysis program the detection thresholds for many elements could be decreased by a substantial amount compared to those using the MLS with conventional analysis.

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Figure Caption

Figure 1. Part of a Germanium gamma-ray spectrum from (top) an 8-hour count of a reactor-activated sample and (bottom) part of a spectrum from the same detector employing a neutron generator in a borehole for 100 seconds.

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