Performance Assessment of a New Gamma Spectroscopy Toolkit: Peak Doctor and the Spectral Nondestructive Assay Platform (SNAP) - 17397

Alan Simpson *, Randy Lucero * * Pajarito Scientific Corp., 2976 Rodeo Park Drive E., Santa Fe, NM 87505, USA asimpson@pscnda.com, rlucero@pscnda.com

ABSTRACT

High resolution gamma spectroscopy (HRGS) is a widely used technique for nondestructive characterization of nuclear materials, and assay of radioactive waste. The ability to accurately evaluate raw spectral data is an important step in producing high-quality results. A spectral analysis application known as Peak Doctor has been developed under a Cooperative Research and Development Agreement (CRADA) between LANL and Pajarito Scientific Corporation (PSC). The software has undergone several years of testing and validation by the Radioactive Waste Characterization Team of the LANL Waste Management Services Group (WM-SVS). PeakDoctor is designed to work with the Spectral Nondestructive Assay Platform (SNAP[™]) to provide a complete HRGS analysis engine. SNAP[™] performs model specific corrections for attenuation and geometry. These applications are the major components of a new toolkit designed primarily for portable far-field nondestructive assay.

Peak Doctor performs a very accurate peak fit analysis with the goal of improving upon the capabilities of existing commercially available routines. It is designed to be user-configurable and can be customized to any given type of detector and any given type of spectrum. Peak Doctor was developed to resolve many of the inherent complexities in gamma ray spectra including overlapping peaks, complex multiplet regions, large step peaks, backscatter regions and Compton edges.

Unlike most spectral analysis platforms, Peak Doctor does not rely on the energy calibration and detector resolution parameters that are saved by the operator in the spectrum file. Instead, key parameters are pre-defined for individual detectors. The software fits a continuum using a series of splines between a series of junctions or "knots". Fitting techniques are used to join the splines together to create a near-continuous multi-element curve. Optimizing the location of the knots is one of Peak Doctor's most powerful features. The knots are initially configured using a pre-defined list and are removed or added automatically during the fitting process. Knots are also created when new features are identified such as Step Peaks and Compton Edges. The user can also manually specify knots in order to improve the continuum fit.

The initial fit is improved on by removing any outlier regions (which are converted to peaks) and the continuum fitting process is repeated. At this stage, an experienced user can work interactively with the fit by manually converting peak regions to continuum or vice versa. The final step is to fit a series of peaks above

the continuum based on detector parameters. Single and multiplet peaks are then processed by either the tailing (piecewise) or non-tailing (Gaussian) Levenberg Marquardt non-linear peak fitting routine depending on the user defined selection. Only a rough knowledge of the detector characteristics (energy calibration and resolution) is required for the fitting process to proceed with good accuracy. Any peaks that are missed can be manually added by the user and will also be fitted. Discontinuities in the peak / continuum fit can be rapidly identified by reviewing the "residuals scale" plot.

For waste streams that are well characterized, it is often the case that routinely encountered spectra will have similar peaks and continuum features. For these cases a handy "One Step" method is available that proceeds in an automated fashion without user interaction.

Peak Doctor has been configured with a set of default spectrum types including plutonium / transuranic waste (including Weapons Grade Pu, Heat Source Pu, Am-241, Am-243 and Np-237), depleted or enriched uranium, nuclear power plant / intermediate level waste (with fission and activation products such as Cs-137 and Co-60) as well as Naturally Occurring Radioactive Materials (NORM). The user can easily add new spectrum types for specific waste streams or other types of radiological / special nuclear materials.

The output from PeakDoctor (including net peak area, centroid energy and a list of minimum detectable activity levels at pre-defined regions) is used by SNAP[™] to complete the data analysis process. Isotope activities are calculated using configurable template-driven geometry and attenuation correction methods. The software accounts for matrix and container wall effects, collimator / angular corrections, detector efficiency (based on calibration curves) and stand-off distance. SNAP[™] uses published algorithms incorporating a series of decision points during its operation to allow the analyst to provide logical input to guide the software during the analysis of each unique spectrum.

The Peak Doctor / SNAP[™] toolkit has been extensively tested and validated under a variety of conditions using "benchmark" reference spectra. Test scenarios reported include HPGe-based measurements of well characterized uranium and plutonium standards and radioactive sources with a variety of different geometries and matrix materials including surrogate drums and boxes.

OVERVIEW OF PEAK DOCTOR

PeakDoctor (PD) is designed to perform specialized peak fitting of the spectral data in gamma spectroscopy acquisition files [1]. Spectra from three file types can be analyzed: CNF, CHN and Ortec SPC files which can contain anywhere from 1024 to 32,768 channels. The software is designed as a stand-alone product that can produce report files that are compatible with PSC's SNAP[™] software. One of the primary advantages of Peak Doctor is that it does not rely on the energy calibration and detector resolution parameters that are saved by the operator in the spectrum file. Key parameters are pre-defined for individual detectors and the software fits a continuum using a series of splines between junctions or "knots". Fitting techniques are used to join the splines together to create a near-continuous multi-element curve. The user may set and optimize the location of the knots which are also created when new features are identified such as Step Peaks and Compton Edges.

PeakDoctor is written in National Instrument's LabVIEW® software language, version 2014 and is configured for application using the Microsoft operating systems, XP, Windows 7 or higher versions. It can be installed on any standalone or networked system. The software was developed under a Cooperative Research and Development Agreement (CRADA) between Pajarito Scientific Corporation (PSC) and LANL. PSC has licensed Peak Doctor and has distribution and development rights to Version 1.1.

Upon initiation of the "load spectrum" function, an automatic peak search algorithm ("Reveal Peaks") is performed. All peaks detected are highlighted and a marker is placed at the maximum of each peak. The non-peak Compton continuum channels are highlighted in a different color. The graphical interface that is presented after a typical (thorium loaded) spectrum has been loaded in shown in Figure 1.

The initial fit is improved by removing any outlier regions (which are converted to peaks) and the continuum fitting process is repeated. At this stage, an experienced user can work interactively with the fit by manually converting peak regions to continuum or vice versa.

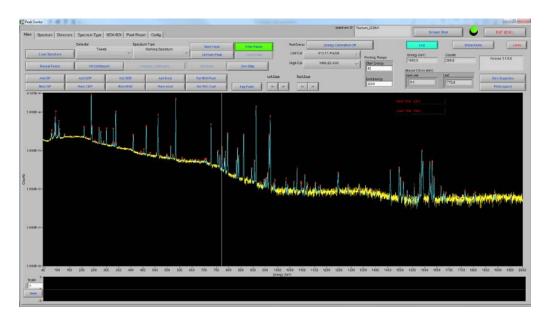


Fig. 1 Thorium Spectrum displayed in Peak Doctor

REFERENCE SPECTRA

A diverse set of reference spectra were used to perform validation testing of Peak Doctor. These spectra range from standard source combinations used for Quality Control tests through to highly challenging spectra with complex features that test the advanced peak fitting capabilities. Table I summarizes the reference spectra. Note that in the "Spectrum Name" the suffix is the unique name of the HPGe detector (e.g. "tweety").

ENERGY CALIBRATION

The operator may choose whether or not to perform an energy recalibration upon loading a spectrum. This module uses a two-point calibration and fits the photopeak centroids of two known peaks to a simple linear equation of the form y = mx + b.

Each reference spectrum was loaded into Peak Doctor utilizing the re-calibration function. It was expected that the calibration adjustment should allow major peaks to be within 1% of the nominal values. Table II shows the energy comparisons for major peaks to the nominal values for a reference spectrum which demonstrates that the Peak Doctor values were within the required tolerance.

DETECTORS AND SPECTRUM TYPE

Prior to loading the spectrum file, the user chooses the detector that created the file from an editable list on the Main page. This provides the program with information about the energy calibration and Full Width at Half Maximum (FWHM) function of the spectrum so that a good approximation of the detector's characteristics is used.

Once the spectral data is loaded, the user chooses a spectrum parameter set (SPS) from the Spectrum Type list. Peak Doctor has been configured with a set of default spectrum types including plutonium / transuranic waste (Weapons Grade Pu, Heat Source Pu, Am-241, Am-243 and Np-237), depleted or enriched uranium, nuclear power plant / intermediate level waste (with fission and activation products such as Cs-137 and Co-60) as well as Naturally Occurring Radioactive Materials (NORM). The user can easily add new spectrum types for specific waste streams or other types of radiological / special nuclear materials.

The SPS contains information that directs the continuum fitting process and assists with the reveal peaks function. This page allows spectrum types to be defined and modified, and stores a fully editable spectrum parameter file that contains the following information: step peaks, Compton edge peaks, backscatter energies, manual knot locations, peak regions, and continuum regions. Figure 2 shows an example spectrum type for Am-241/Cs-137 analysis.

Spectrum Name	Туре	Description	Energy Cal. (keV/ch)	Analysis Range (keV)	Count Time (s)
bkgd_tweety	chn	Medium to small peaks from background radiation on a relatively smooth continuum.	0.25	40 - 2000	14400
Thorium_32201A	spc	Peaks from Th-232 and its decay chain.	0.25	40 - 2000	1800
Eu_Am_Q2	cnf	Eu-152 and Am-241.	0.25	40 - 2000	900
QC_source_tweety	chn	A Quality Control (QC) Spectrum with two prominent step peaks: Am-241 at 59.5 keV and Cs-137 at 661.7 keV.	0.25	40 - 670	300
WGPu_tweety	chn	Weapons Grade Pu with multiplet regions and step peaks. Typical radionuclide gamma ray signal from TRU waste containers.	0.25	129 - 430	900
DU_homer	chn	Depleted uranium spectrum. A material frequently encountered in field measurements.	0.25	40 - 2000	2400
HEU_taz	chn	Highly enriched uranium (HEU) spectrum with a huge step peak at 185.7 keV and several multiplet regions. The short count time adds the additional challenge of fitting a continuum to a limited amount of data in the high energy regions.	0.125	117 - 1020	60
Np_taz	chn	Np-237 spectrum with several step peaks and a significant backscatter peak from the 312 keV gamma line.			600
tailing_WGPu	chn	WGPu spectrum with high-dead time (31.33%) taken at nearly 18,000 cps. Provides a test of the low-energy tailing correction.	0.313	120 - 430	60

TABLE I. Reference	spectra user	1 for Peak	Doctor	Validation	Testina
INDEL I. NOICICICI	spectra used		DOCIO	vanuation	resting

TABLE II. Comparison of major peak energies to nominal values for spectrum bkgd_tweety.chn

Nuclide	Nominal Energy (keV)	Peak Doctor Energy (keV)	% diff
U-235	185.74	185.72	0.01%
Pb-212	238.58	238.58	0.00%
Pb-214	351.87	351.87	0.00%
Bi-214	609.31	609.26	0.01%
Ac-228	911.21	911.17	0.00%
K-40	1460.83	1460.83	0.00%
Bi-214	1764.49	1764.48	0.00%

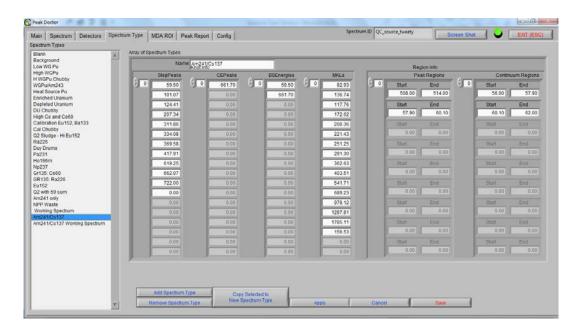


Fig. 2 Example spectrum type (for Am-241/Cs-137).

FIT CONTINUUM AND IMPROVE CONTINUUM

The Fit Continuum function performs a linear least squares fit to a cubic spline on the background continuum that lies underneath the peaks. Peak and continuum regions are determined from the peak search algorithm and the software compares the value of the continuum splines to the spectrum, channel by channel. The difference is normalized to the square root of the continuum fit and then plotted to populate the residuals scale.

The Improve Continuum function converts all channels in the spectrum that are considered part of the continuum, yet exceed the residuals scale by 3 sigma or more, to peak channels. The continuum is then refit. Testing was performed using several spectra from multiple detectors containing a variety of spectrum types.

PEAK FITTING

The final step in Peak Doctor's analysis is to fit a series of peaks above the continuum based on detector parameters. Single and multiplet peaks are then processed by either the tailing (piecewise) or non-tailing (Gaussian) Levenberg Marquardt non-linear peak fitting routine depending on the user defined selection. Only a rough knowledge of the detector characteristics (energy calibration and resolution) is required for the fitting to proceed with good accuracy. Any peaks that are missed can be manually added and will also be fitted. Discontinuities in the peak / continuum fit can be rapidly identified by reviewing the "residuals scale".

The peak fits make use of the FWHM information present in the "Detectors" module and the results of the initial peak search algorithm. The peak fits are visually displayed in the spectrum view and the residuals scale. Two files are created during this routine, a PRN file which contains a peak report detailing the characteristics of the peaks fit (centroid energy, FWHM, net area, net area uncertainty and background area) and a REV file that allows a reviewer to examine the spectrum peak fits and continuum fit at a later time. An example is shown in Figure 3.

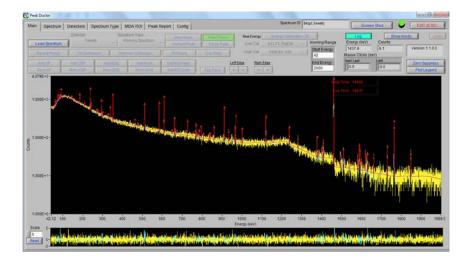


Fig. 3 Peak analysis of spectrum bkgd_tweety.CHN

The Fit Peaks routine was applied to several spectra (with and without tailing) from multiple detectors with a variety of spectrum types. It was verified that the PRN and REV files were created properly.

"ONE STEP" FEATURE

For waste streams that are well characterized, it is often the case that routinely encountered spectra will have similar peaks and continuum features. For these cases a handy "One Step" method is available that proceeds in an automated fashion without user interaction.

MDA (CONTINUUM) ANALYSIS

A Minimum Detectable Activity (MDA) analysis is performed on the spectrum. The MDA uses the sum all the counts in the spectrum over +/- 1 FWHM from the centroid. The MDA nuclide list (nuclide name, gamma-ray energy and yield) is fully editable so that new gamma-ray peaks can be added or deleted as desired. A report is produced in a SNAP[™] RPU text file format that lists the net peak area (zero if no peak present) and the sum of the continuum counts for the MDA region.

VALIDATION TESTING

There are two fundamental sets of results which validated using an Excel version of Peak Doctor: 1) the FWHM, and the net area, in the PRN file, and 2) the continuum

values from the MDA routine that in the RPU report file. Validation was performed with side by side comparisons of all healthy-sized (>1000 counts in most cases) peaks in each of six spectra. The results of testing are given in Table III. The Excel version has been verified and validated previously [2].

Energy

The centroid energy of fitted photopeaks should be accurately calculated for a good peak fit to occur. This function was tested against a criterion of \pm 1% variation. Table II shows the comparisons of calculated photopeak energies in the six test spectra. In all cases the energies compare very closely with the largest deviation being -0.76% and all within the stated accepted criterion.

Full Width at Half Maximum

The FWHM values impact the net area that is calculated for the peak. This function was tested against a criterion of \pm 5% variation. There was a total of 6 cases out of 73 peaks in which the FWHM comparison was more than +/-5% different. In each case the discrepancies were evaluated and considered to be acceptable.

Area

The net counts of the photopeak are the most important results as these are used directly in activity calculations. In most cases, photopeaks with more than 1000 net counts should have a relative standard deviation of 5% or less. The exception to this is for spectra where there is a large continuum that boosts the relative uncertainty in most of the net peak areas. The acceptance criterion was for photopeaks that have greater than 1000 net counts (or greater than 3000 for high continuum spectra) to agree within +/-5%. For discrepancies greater than 5%, an attempt was made to identify the cause the cause and evaluate the implications to validation. There was a total of 13 cases out of 73 peaks in which the net area comparison was more than +/-5% different.

In most of these cases, the PD net area was lower than the Excel net area (9 out of the 13) and the FWHM used to evaluate the Gaussian fit was lower. It would be expected that a smaller FWHM would result in a smaller integrated Gaussian. Small differences in the net area of the PD version are acceptable because it has already been demonstrated that the PD FWHM calculations are equivalent to the Excel values. In all these cases the PD residual was under 3 sigma indicating a good peak fit. Only one case that was outside 10% difference: the 143.5 keV Np-237 peak which is discussed above. The other peaks exceeding 5% difference were all part of multiplets and, after evaluation, these discrepancies were considered to be within PD's expected performance envelope.

Minimum Detectable Activity

A slightly different approach is used for MDA validation because the continuum values can come from any part of the spectrum. The criterion was for the two sets of values to fall within 2 standard deviations from one another. This was confirmed for all of the test spectra and therefore this function of PD has been validated. Table III. Validation Test Results for Background and QC Spectra

Spec ID	Excel Energy (keV)	PD Energy (keV)	Energy % Diff	Excel FWHM (keV)	PD FWHM (keV)	FWHM % Diff	Excel Net Area (counts)	PD Net Area (counts)	Area % Diff
Bkg	77	77.12	0.16%	0.693	0.68	-1.88%	1055	1017	-3.60%
Bkg	92.41	92.52	0.12%	0.958	0.92	-3.97%	3164	3002	-5.12%
Bkg	185.69	185.78	0.05%	0.932	0.94	0.86%	2507	2530	0.92%
Bkg	238.56	238.64	0.03%	0.869	0.86	-1.04%	5993	5895	-1.64%
Bkg	241.76	241.88	0.05%	1.408	1.32	-6.25%	1594	1496	-6.15%
Bkg	295.12	295.2	0.03%	0.9	0.91	1.11%	2580	2602	0.85%
Bkg	338.25	338.31	0.02%	0.959	0.96	0.10%	1376	1367	-0.65%
Bkg	351.86	351.92	0.02%	0.993	1	0.70%	5009	5077	1.36%
Bkg	510.86	510.87	0.00%	2.362	2.21	-6.44%	5733	5522	-3.68%
Bkg	583.18	583.2	0.00%	1.17	1.18	0.85%	3840	3890	1.30%
Bkg	609.29	609.3	0.00%	1.239	1.24	0.08%	6099	6087	-0.20%
Bkg	661.73	661.73	0.00%	1.269	1.27	0.08%	1165	1182	1.46%
Bkg	911.26	911.2	-0.01%	1.434	1.43	-0.28%	3522	3497	-0.71%
Bkg	969.06	968.99	-0.01%	1.455	1.44	-1.03%	2147	2109	-1.77%
Bkg	1120.45	1120.35	-0.01%	1.712	1.7	-0.70%	2246	2230	-0.71%
Bkg	1461	1460.83	-0.01%	1.826	1.83	0.22%	29562	29520	-0.14%
Bkg	1764.7	1764.47	-0.01%	2.043	2.06	0.83%	2228	2231	0.13%
QC	59.54	59.54	0.00%	0.701	0.71	1.28%	3549	3592	1.21%
QC	661.65	661.69	0.01%	1.286	1.29	0.31%	5244	5250	0.11%

Tailing

The Levenberg–Marquardt (LMA) algorithm [3] used for non-linear least squares fitting was evaluated in PD and Excel. The tailing fits were explicitly evaluated using the LMA function with a criterion of achieving identical results. The spectrum WGPu_detK.chn was used to qualitatively evaluate the goodness of fit for tailing by visual examination of the graphed curve fit and of the residual. Comparison to the same fits using strictly a Gaussian was part of this evaluation.

Figures 4 and 5 shows the fit for the 2224 keV peak with the tailing function off (strictly Gaussian) and on respectively. For the "tailing off" case, visual inspection reveals that the Gaussian is missing some of the tailed left edge of the peak. The

residual is also slightly greater than 3 on that edge and higher than the rest of the residual also indicating a poor fit on that edge. Whereas for the "tailing on" case, visual inspection reveals that the tailing function has captured the tailed left edge of the peak (as indicated by the white pointer in the figures). The residual is also much improved on that edge.

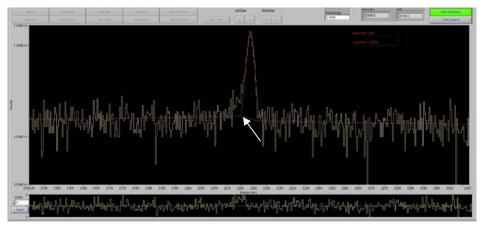


Fig. 4 The 2224keV peak fit with the tailing function OFF

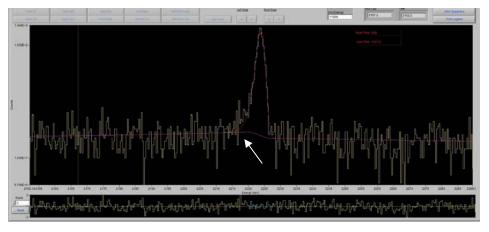


Fig. 5 The 2224keV peak fit with the tailing function ON

Background Counts and Area Uncertainty

The reported "background" represents the counts under the continuum for +/- 0.5 FWHM width of spectrum centered on the peak centroid. The uncertainty in peak area is defined as $\sqrt{(\text{Area}+4\times\text{Background})}$. An independent calculation of these values was performed in Excel from analysis of spectrum bkgd_tweety. All uncertainties agreed to within machine rounding precision and are therefore validated.

Validation Summary

The FWHM, peak fitting, area calculation, MDA and tailing functions for PD has been tested and validated. For the area calculation all discrepancies greater than +/-5% are understandable and do not compromise the validity of the PD calculation.

SPECTRAL NONDESTRUCTIVE ASSAY PLATFORM

SNAP[™] is a spectral analytical software program originally developed by Eberline Services and now owned and distributed by Pajarito Scientific Corporation [4]. The program uses gamma spectral data from a counting system to produce assay results for any geometry and matrix. The analyst can perform peak identification, source modeling, and assay calculations interactively with the program. Experience from end users has demonstrated that SNAP[™] offers accuracy and sensitivity comparable to state-of-the-art measurement systems such as segmented gamma scanners [5, 6, 7, 8, 9].

The output files (PRN and RPU) from PeakDoctor (including net peak area, centroid energy and a list of minimum detectable activity levels at pre-defined regions) are used by SNAP[™] to complete the data analysis process. Nuclide activities are calculated using configurable template-driven geometry and attenuation correction methods. The software accounts for matrix and container wall effects, collimator / angular corrections, detector efficiency (based on calibration curves) and stand-off distance. SNAP[™] uses published algorithms incorporating a series of decision points during its operation to allow the analyst to provide logical input to guide the software during the analysis of each spectrum.

SNAP[™] supports multiple detectors and is capable of importing report files from a wide variety of commercially supplied formats. The software executes the peak ID process in a real-time interactive mode allowing the data analyst to identify coincidence peaks, single or double escape peaks, multiplets, prompt gamma-rays, and fluorescence x-rays. An intrinsic efficiency calibration can be used for modeling a diverse range of geometries.

Configuration Modelling

The analyst can model the field measurement configuration (source and detector geometry) and may choose one of many standard containers (e.g. boxes or cylinders/drums) for repetitive measurements or create and store alternate configurations (Figure 6). In addition, modeling of line or plane sources is possible from the main modelling page or the user can create a custom geometry or source distribution using a "Special Modelling" mode (also shown in Figure 6).

SNAP[™]'s uses a point-kernel method with a matrix of distributed points within the volume of the item being modeled. The analyst may weight any and all of the 1,920

points in the array as required. So a known activity density profile can be simulated if material is located, say on a particular surface or at the bottom of a container.

Various matrix contents can also be simulated. A customizable materials library is used to calculate mass attenuation coefficients for typical material types encountered in field measurements. In addition, attenuation losses in air are corrected for, which is especially important at low energies and when the distance between the container and the detector is significant.

Differential Peak Analysis

A graphical differential peak analysis interface (Figure 7) is used to view plots of relative activities at different energies (a very powerful analytical tool). For each nuclide of interest, the calculated activity of each peak relative to its average activity is displayed allowing the analyst to validate, refine and improve the accuracy of the modelling approach used.

Self-attenuation in lumps can be corrected for using an in-built analytical model. The analyst can adjust the size (in microns) of a uranium or plutonium particle to see the effect that lump size has on the differential peak analysis.

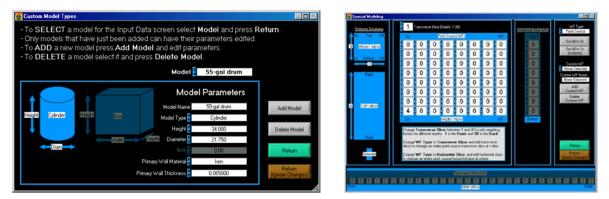


Fig. 6 Creating Custom Models and Special Modelling Interface

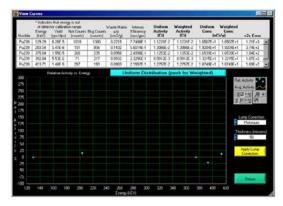


Fig. 7 SNAP[™] Graphical Differential Peak Analysis Interface

Transmission Corrections

Data from gamma-ray transmission measurements may be used as an alternative to modeling the matrix attenuation losses. This method is best applied when limited information is available regarding the matrix-attenuation effects.

TMU and MDA Analysis

A detailed Total Measurement Uncertainty (TMU) analysis (including errors from attenuation and geometry assumptions, statistical error, and detector efficiency error) is supported. Error propagation is performed based on geometrical and matrix effects, counting-statistics and detector calibration uncertainty. All these errors are summed in quadrature to give a final TMU for each reported activity.

MDA calculations are performed on user-selected nuclides and energies, supporting standard regulatory reporting methods. The MDA analysis is compatible with the Peak Doctor RPU output file which provides the continuum counts at specified regions of interest.

Uranium and Plutonium Isotopic Analysis

SNAP[™] can also perform isotopic analyses for uranium and plutonium based on the relative-efficiency curve. The limitation of this technique is that all the nuclides in the emission source must be uniformly mixed together. The user must take care to properly deconvolve the overlapping peaks using advanced spectral analysis software such as Peak Doctor.

Rate Loss Correction

The software includes a provision for rate-loss (dead-time) correction. Rate loss is a decrease in photopeak counting efficiency at high gamma flux from an emission source to the detector, which usually results from coincidence summing of photopeaks. The rate-loss correction factor is measured during gamma counting or can be calculated based on percent detector dead time.

Reporting

After completion of spectral analysis and calculation, a report is generated that summarizes the radionuclide assay and model input parameters. The acquired data from background and emission source measurements and the results of radionuclide identification are reported in separate files, but can be attached to the summary report as deemed appropriate.

Application Areas

SNAP[™] is ideal for power plants, decommission of facilities, waste assay, universities, and any situation where analysis of complex spectra is required. The software is normally used in conjunction with a portable far-field detection system comprising a detector, electronics, cart and suitable collimator / shield.

Applications of SNAP[™] to date include low-level and transuranic drum assay at Los Alamos National Laboratory [5,6], enriched uranium waste assay at the Atomic Weapons Establishment in the UK [7, 8], assay of large waste boxes [10], sludge characterization [11], and screening of empty waste drums [12]. These measurements have supported final disposition, segregation and sentencing of a variety of waste streams into appropriate facilities including TRU waste at the Waste Isolation Pilot Plant (WIPP).

CONCLUSIONS

The ability to accurately evaluate raw spectral data is an important step in producing high-quality gamma spectroscopy results. A spectral analysis application known as Peak Doctor has been developed by LANL and Pajarito Scientific Corporation (PSC) and has undergone several years of testing and improvement.

Validation tests have confirmed that Peak Doctor performs a very accurate peak fit analysis and can provide improved capabilities for data analysts compared to existing commercially available routines. It is user-configurable and adaptable for any type of detector and any given type of spectrum. Peak Doctor can resolve many of the inherent complexities in gamma ray spectra including overlapping peaks, complex multiplet regions, large step peaks, backscatter regions and Compton edges.

PeakDoctor works with the Spectral Nondestructive Assay Platform (SNAP[™]) to provide a complete HRGS analysis engine. These applications form the major components of a new toolkit for portable far-field non-destructive assay. SNAP[™] performs the necessary model specific corrections for attenuation and geometry. The analyst can perform source distribution and matrix modeling interactively with the program to improve the accuracy of the activity calculations. The performance of SNAP[™] used together with portable far-field detection system has been demonstrated to be comparable to more complex fixed-installation systems such as segmented gamma scanners.

REFERENCES

- 1. User Manual for LabVIEW® PeakDoctor Version 1.1, Pajarito Scientific Corporation, PSC-4008-UM-001, April 2014
- "Validation of Peak Doctor, RobWin, and Maestro Gamma Ray Spectrum Fitting Software Routines" REPORT-SWO-034, R.0, Los Alamos National Laboratory, February 2004.

- 3. D. Marquardt "An Algorithm for Least-Squares Estimation of Nonlinear Parameters". SIAM Journal on Applied Mathematics 11 (2): 431–441, (1963).
- 4. SNAP[™] User Manual, Pajarito Scientific Corporation, 2016
- K. Gruetzmacher, S. Myers, "Comparison of Waste Matrix Attenuation Corrections using Gamma-Ray Transmission Measurements vs a Mathematical Modeling Approach", Waste Management, WM'00, February 2000, Tucson, AZ
- 6. K. Gruetzmacher, S. Myers, "Low-Level Waste Drum Assay Inter-Comparison Study", WM'03, February 2003, Tucson, AZ
- 7. T.J. Miller, "Applications where SNAP is BPM for Radioactive Waste Assay", WM'08, Phoenix, AZ, February 2008,
- 8. T.J. Miller, "Enriched Uranium Waste Assay at AWE", Waste Management, WM'09, Phoenix, AZ, March 2009.
- 9. "NPL Waste Drum Inter-Comparison Study Workshop", London, UK, September 2007
- S. Myers, K. Gruetzmacher, C. Sheffing, L. Gallegos, R. Bustos, "Practical Gamma Spectroscopy Assay Techniques for Large Volume Low-Level Waste Boxes", Waste Management, WM'02, Tucson, AZ, February 2002
- K.M. Gruetzmacher, R.M. Bustos, S.G. Ferran, L.E., Gallegos, R.P. Lucero, "WIPP WAC Equivalence Support Measurements for Low-Level Sludge at Los Alamos National Laboratory", Waste Management, WM'12, Phoenix, AZ, February 2012.
- K. M. Gruetzmacher, R. M. Bustos, S. G. Ferran, L. E. Gallegos, R. P. Lucero, "Screening and Spectral Summing of LANL Empty Waste Drums", Waste Management, WM'13, Phoenix, AZ, February 2013.

ACKNOWLEDGMENTS

The authors wish to acknowledge Los Alamos National Laboratory as co-developers of the Peak Doctor application and for provision of spectral files used in the testing and validation. Acknowledgment is also given to the technical support provided by the Scott Garner of LANL and for his work in the development and testing of Peak Doctor. Steve Myers of LANL is acknowledged for his work in the development and testing of SNAP[™]. Kathleen Gruetzmacher and her supporting team members at LANL are acknowledged for their work in technical support, development and testing of this toolkit.