Programs and Procedures for Assessing Quality of Spectral Gamma-Ray Borehole Data for the UGTA

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Introduction

This report describes the procedures and computer programs used to process spectral gamma-ray borehole logging data in the UGTA (UnderGround Test Area) program at the NTS (Nevada Test Site) to assess data quality. These programs and procedures were used to analyze data from five boreholes in the UGTA program.¹⁻⁵ Development of these computer programs and procedures required considerable effort and the primary purpose of this report is to provide continuity with future activities related to spectral gamma-ray borehole logging in the UGTA program. This is especially important because of the long time interval between cessation of logging in April, 1996 and the next round of activity, which has not yet occurred. This report should also be useful if any quality control issues arise regarding past or forthcoming spectral gamma-ray log analyses.

In the characterization work underway at the Nevada Test Site Underground Test Area, the logging contractor, Western Atlas, agreed to identify five artificial nuclides based on their gamma-ray signatures. Those nuclides are ^{60}Co (cobalt-60), ^{106}Ru (ruthenium-106), ^{125}Sb (antimony-125), ^{134}Cs (cesium-134), and ^{137}Cs (cesium-137). In the case of ^{106}Ru , which is not a gamma emitter, any detected gamma rays come from the daughter nuclide ^{106}Rh (rhodium-106) which has a half-life of 30 s. With such a short half-life, ^{106}Rh can be considered to be in equilibrium with ^{106}Ru under most conditions so the result is the same as if the gamma rays were emitted by the ^{106}Ru .

The Western Atlas spectral gamma-ray curve plots from a given borehole present detailed qualitative information on the apparent distribution of natural and artificial nuclides with depth in the borehole. The computer programs and procedures described in this report were used to provide a quality analysis of the contractor's processed data and to work with the contractor to validate and/or refine their existing automatic processing. This was done using a procedure that was developed and tested successfully in earlier work at the NTS⁶; the revised and updated procedure is documented in this report.

The former name of Western Atlas was Atlas Wireline Services or AWS, and those initials still appear occasionally in program documentation or variable names.

Characteristics of the logging system

Western Atlas does not attempt to provide a quantitative radioelement concentration estimate for the artificial nuclides. Log curves are expressed in counts per second attributed to each nuclide and additionally, for the artificial nuclides, as a per cent of the total count rate attributed to K, U, and Th. Although the Atlas logging tool is characterized for five artificial nuclides, other artificial gamma emitters may be present in a given borehole depending on the type of underground test and the elapsed time since the test was executed. For example, one artificial nuclide not included in the Atlas tool characterization was detected in the water samples from ER20-6 #1, $^{102\text{m}}\text{Rh}$ (rhodium-102 metastable).³

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The Western Atlas spectral gamma-ray tool used in the Nevada Test Site Underground Test Area work to date has a 2 in by 12 in CsI(Na) (sodium-doped cesium iodide) scintillation detector. Cesium iodide has lower energy resolution than the better known sodium iodide scintillation material but is more rugged and is also more efficient, giving higher count rates especially at higher energies and potentially better counting statistics. Detected gamma rays are sorted into 256 energy bins using a pulse-height analyzer in the tool and the data are transmitted up the logging cable in digital form. Western Atlas personnel perform an energy calibration before and after each logging run using a calibration source. Atlas also performs a running adjustment of the spectral energy scale during the office post-processing based on the positions of known peaks in the naturally occurring spectral components; this will be discussed below.

The logging system has been characterized by Western Atlas so that, at least in theory, the five artificial nuclides listed above can be identified based on their gamma-ray signatures. Atlas does not attempt to provide a quantitative radioelement concentration estimate for the artificial nuclides. Log curves are expressed in counts per second attributed to each nuclide and additionally, for the artificial nuclides, as a per cent of the total count rate attributed to K, U, and Th.

Spectral gamma-ray logging is potentially very sensitive, giving an estimated detection threshold better than 0.1 pCi/g for ^{137}Cs under good conditions. However, the conditions at the NTS are not ideal. At the NTS, the decision was made to use a scintillator-based logging system for operational reasons, in part because logging with high-resolution detectors would be much more expensive. With scintillator-based systems, much depends on the contractor's ability to extract subtle information from noisy, low-resolution gamma-ray spectra.

In previous reports⁽¹⁻⁵⁾ we documented several problems with the Western Atlas equipment and procedures that are generally unimportant in the normal use of that system in petroleum logging, but can cause problems when searching for artificial gamma emitters. In 1996, we conducted joint experiments with Atlas at their research facility in Houston to see what effect these deficiencies might have on the results. We found that for experimental conditions that were essentially the same as the calibration conditions, the data processing worked well. As conditions departed from this ideal, errors increased. In general, the processing was able to identify the artificial nuclides that were actually present in any given experiment, but frequently also identified nuclides, sometimes indicating substantial quantities, that were not present. The system is able to recognize the presence of artificial nuclides fairly reliably, but sometimes misidentifies the specific constituents. Such errors are probably an unavoidable consequence of trying to extract small signals from noisy data but steps can be taken to reduce the errors. The contractor seems to be following generally accepted professional practice although some improvements are possible. Some of the deficiencies are discussed briefly below.

Energy calibration. While the energy calibrations of the spectral templates are not bad, there is room for improvement. Errors in peak position of a channel or two are common. We also have identified a separate problem with the Atlas automatic peak tracking where photopeaks from artificial nuclides interfere with the natural reference peaks used for post-processing calibration on the fly. Thus, the spectral calibration can be at its worst in zones of greatest interest in the UGTA work, zones that are contaminated by artificial gamma emitters.

Incorrect borehole environment. The borehole environments at the calibration facilities in which the Western Atlas spectral gamma-ray logging system was characterized differ significantly from

the actual borehole environment in the Underground Test Area work. This results in different spectral shapes that can adversely affect the processing.

Missing templates. Artificial gamma emitters may be present in significant quantities that are not included in the data processing; this could lead to erroneous nuclide identifications. Water samples from borehole ER-20-5 #1, for example, indicated two europium isotopes that are prolific gamma emitters in the energy range for which the Western Atlas logging system is sensitive, but for which spectral templates are not available.¹

Differential non-linearity. Pronounced differential non-linearity was observed in the Western Atlas spectra; in our experience, the differential non-linearity is unacceptably high for addressing the difficult problems at the NTS.

Sensitivity to logging speed variations. The field prints produced for borehole ER-20-6 #3 contained errors (false anomalies) in the API curve due to logging speed variations. These would probably be eliminated if the contractor were to convert the data from counts to counts per second before plotting. The post-processed data do not contain these errors.⁵

Missing repeat run data. Our quality control activities were limited for borehole ER-20-5 #3 by the unavailability of processed repeat run data, as discussed in the main body of this report. Repeat run data are important at various stages of log analysis and quality control and we recommend that delivery of such data by the logging contractor be a routine part of any future contract.

Sensitivity of results to post-processing procedure. In the analysis of data from borehole ER 20-5 #1 reported earlier,¹ we noted that Western Atlas had supplied at least two sets of data processed on two different dates more than two months apart. A comparison of those two data sets showed substantial differences in the apparent artificial nuclide anomalies. No explanation was given in the log headers to explain these differences, which seem to illustrate the sensitivity of the artificial nuclide concentrations to the post-processing procedure. In the joint experiments conducted in Houston late in FY96, we found that relatively small adjustments in processing parameters such as energy calibration produced variations in the processed data similar to those shown in these examples. Sometimes, carefully optimizing the processing parameters actually made the results worse. While this does not bolster confidence in the results, it does emphasize the fact that small anomalies – those not flagged as statistically significant – should not be relied upon as being “real.”

Programming language

The computer programs developed for spectral gamma-ray log analysis and quality control for the UGTA project were written in the MATLAB programming language, version 4.2b. MATLAB (MATrix LABoratory) is a high-level language well suited to R&D work where fast development of programs that may only be used a few times is important. The basic data element is a matrix that does not require dimensioning and MATLAB is very efficient for operations on an entire array at once.

Obviously, some familiarity with MATLAB is required to maintain and modify these programs; the good news is that for a person with moderate programming experience, a day or two of work with MATLAB should be enough to become productive. Aficionados of elegant programming may be disappointed by the in-line code encouraged by MATLAB and found in these programs. Similarly, because of the limited amount of use these programs were intended to receive, we developed them using a pragmatic approach, so they have the flavor of expedient R&D programs rather than polished production programs. We apologize if this makes anyone's job more difficult; it made

ours easier. Still, our aim has been to include enough documentation inside the programs to make them understandable. This includes comments scattered through the programs as well as descriptive variable names. MATLAB allows long variable names so we have used names like InputFileID, TotalTime, and NormalizedSpectrum to make the programs easier to follow.

MATLAB source files used for the data processing are called M-files and have a ".M" file extension, such as CALSPEC.M. In this report, program names are frequently given without the ".M" file extension but this file extension should be assumed by the reader for all source files. Data files and parameter files have other file extensions, as will be described.

User qualifications

As discussed above, prior experience with the MATLAB programming language is not necessary to use these data analysis and quality control programs because the language is not difficult to learn for anyone with moderate programming experience. Appropriate tests can be devised by the user to ensure that the programs are performing as expected. However, a good background in gamma-ray spectral analysis is essential. If the computer programs presented here are used simply as canned programs by a person with inadequate background in the appropriate physics, the results will probably not be satisfactory.

Form of the data

The field data were supplied by the contractor in *computed log curve data files* and *full spectral data files*. Each computed log curve data file starts with a header containing a variable number of lines of information describing factors such as the borehole, operator, logging system, logging runs, and the names and brief descriptions of the computed log curves contained in the file. The header is followed by the data section containing one data record for each depth at which a measurement was obtained in the borehole, at quarter-foot intervals in the case of the UGTA work. Each data record contains the current depth and values for twenty raw and/or computed log-related parameters as described in Table 1.

The full spectral data files start with a short header containing the file name, customer name (DOE), borehole name, log date, and information describing the logging depth range and sample interval. This header is followed by the data section containing one data record for each depth at which a measurement was obtained in the borehole. Each data record begins with the current depth and the sample time for this measurement, followed by 256 integer numbers, each corresponding to the number of counts accumulated in the respective spectral channel.

In addition to the field data described above, the contractor supplies *spectral template data files* containing 256-channel spectral *templates* or reference spectra developed under controlled conditions. Contractor personnel process the spectral gamma-ray field data using a least-squares fit of these spectral templates to extract the contributions of the various gamma-emitting nuclides. For the UGTA work, the contractor used and supplied eight templates representing the three naturally-occurring radioelement families (^{40}K , the natural uranium isotopes and daughters, and natural thorium and its daughters) along with five artificial nuclides (^{60}Co , ^{106}Ru , ^{125}Sb , ^{134}Cs , and ^{137}Cs). Each spectral template is an experimental spectrum obtained in a model borehole containing a particular gamma-emitting nuclide or nuclide family in a particular geometrical configuration. Each template file supplied by the contractor for the UGTA work contains 18 data blocks in sequence. Each block of data describes a given combination of source nuclide and geometrical

Table 1. Depth-dependent log parameters recorded in the computed log curve data files.

PARAMETER	DESCRIPTION
DEPT	Depth of the measurement point (feet).
GR	Computed gross count gamma ray (API units).
KUTH	Potassium + uranium + thorium (API units).
COC	Total countrate in ^{60}Co window (counts/s).
CS4C	Total countrate in ^{134}Cs window (counts/s).
CS7C	Total countrate in ^{137}Cs window (counts/s).
RUC	Total countrate in ^{106}Ru window (counts/s).
SBC	Total countrate in ^{125}Sb window (counts/s).
KC	Total countrate in ^{40}K window (counts/s).
THC	Total countrate in ^{232}Th family window (counts/s).
UC	Total countrate in ^{238}U family window (counts/s).
COP	Countrate in the ^{60}Co window as a percentage of the combined countrates in the potassium, uranium and thorium windows.
CS4P	Countrate in the ^{134}Cs window as a percentage of the combined countrates in the potassium, uranium and thorium windows.
CS7P	Countrate in the ^{137}Cs window as a percentage of the combined countrates in the potassium, uranium and thorium windows.
RUP	Countrate in the ^{102}Ru window as a percentage of the combined countrates in the potassium, uranium and thorium windows.
SBP	Countrate in the ^{125}Sb window as a percentage of the combined countrates in the potassium, uranium and thorium windows.
QMSL	Multiplicative energy calibration factor or gain, M (channels/MeV).
QASL	Additive energy calibration factor or offset, A (channels).
QPKS	Number of specified spectral reference peaks recognized by the calibration routine (out of a possible 5 peaks). Normally QPKS must be at least 4 for an automatic recalibration to be performed.
QCAL	Slope of the line obtained by performing linear regression on a plot of measured reference peak channels (y-axis) against expected reference peak channels (x-axis).
QSA	Chi-squared value describing goodness-of-fit of the reference peak channels versus energy plot. Normally, QSA must be less than 1 for an automatic recalibration to be performed.

Table 2. Data order for each of the data blocks representing the 18 spectral templates.

PARAMETER	DESCRIPTION
1	Atomic weight of nuclide or nuclide family used for identification purposes (integer)
2	Borehole casing type (1 = casing, 0 = no casing, 999 = unknown)
3	Borehole fluid type (0 = air, 1 = water, 2 = mud, 999 = unknown)
4	Source distance into formation from borehole wall in inches (0=source in borehole, 999=distributed)
5	Multiplicative spectral calibration factor or gain, M (channels/MeV)
6	Additive spectral calibration factor or offset, A (channels)
7	256 channel spectrum (32 rows of 8 columns)
8	Accumulation time

Table 3. Each of the 18 data blocks in each spectral template data file corresponds to a particular nuclide under various geometrical conditions; the nuclides are listed in this table.

Block(s)	1	2	3	4-6	7-9	10-12	13-15	16-18
Nuclide	⁴⁰ K	²³⁸ U	²³² Th	¹²⁵ Sb	¹⁰⁶ Ru	¹³⁷ Cs	¹³⁴ Cs	⁶⁰ Co

configuration as described in Table 2. The order of the 18 blocks in each template data file is given in Table 3. Note that there are three templates for each artificial nuclide just as described in Table 3. These three templates (for example, templates 4-6 for ¹⁰⁶Ru) represent three different calibration environments: (a) the logging instrument in a simulated borehole in a sandstone block with a button calibration source located 3 in inside the borehole wall in a small hole drilled from the outside of the block, (b) as above but with a button calibration source located 1 in inside the borehole wall, and (c) the logging instrument hanging in air with the button source about 13 in from the pressure housing. Western atlas personnel routinely use the template made with the source 1 in inside the borehole wall (case b, above) to represent each artificial nuclide spectrum, concluding that these calibration spectra seem to represent the best fit to the field data.

Western Atlas quality control parameters

In the Western Atlas spectral gamma-ray log post-processing, an initial calibration spectrum is summed over the first 50 ft of log. Quality control tests and calibration adjustments, if any, are based on that summed spectrum for a point centered in that 50 ft section. As processing proceeds, spectra from successive sample depths are added into the calibration spectrum and spectra are

subtracted at the same rate from the other end of the 50 ft interval so the calibration spectrum always represents a spectrum accumulated over a 50 ft interval centered on the current depth.⁽³⁾ The quality control parameters are described briefly in Table 1.

For an automatic spectral recalibration (adjustment of QMSL and QASL) to take place, Atlas requires certain criteria to be met (generally QPKS = 4 and QSA < 1). Unless these criteria are met the energy calibration factors QMSL and QASL remain fixed. Unfortunately, we found the automatic spectral recalibration routine was influenced adversely by interference from artificial gamma emitters, that is, artificial nuclide photopeaks were incorrectly identified as nearby natural nuclide photopeaks for which the recalibration routine searches. This erroneous spectral calibration reduces the chance that the Atlas automatic full-spectral processing software will correctly determine which artificial nuclides are actually present and which are not. Because we did not consider the energy calibration values for this log reliable, each summed field spectrum was individually recalibrated interactively during the analysis.

Data processing procedure

The overall data processing procedure is shown schematically in flow chart A1 (Appendix A). Flow charts are also given for the five principal computer programs used in the routine data processing for log analysis and quality control.

1. *Manual operations.* To begin the processing, the log analyst performs a quality assessment of the field data plots supplied by the contractor (historically these plots are called "bluelines" because at one time they were produced by a blueprint process). The field spectral data file and computed curve data file are then edited manually, if necessary, so the start and stop depths are the same in both. The number of header lines in the curve file is adjusted manually to 100 lines, generally by adding dummy lines.

2. *Run the program PLOT_M_A:* This program reads the Western Atlas curve data file and plots QPKS, QMSL, and QASL (described in Table 1) against depth, along with the five artificial nuclide log curves.

3. *Run the program PLTCURVS:* This program reads the Western Atlas curve data file and plots specified curves against depth. The number of curves plotted, which curves they are, and their order on the plot page are all easily changed. Normally, the program is used to plot curves nominally corresponding to Co-60, Cs-134, Cs-137, Ru-106, Sb-125, K-40, Th family, and U family. These plots are useful for reference in conjunction with the plots produced by PLOT_M_A.

4. *Run the program CALSPEC.* This program adjusts the gain and offset of the recorded field spectra by rechannelizing each spectrum automatically based on the gain (M) and offset (A) values computed by Western Atlas during the post-processing and tabulated in the corresponding curve data file as a function of depth. The purpose of this step is to compensate for gain and offset changes during the logging operation so that, say, the 1.41 MeV 40K peak always appears in a particular channel of the 256-channel spectrum. This is necessary because the energy scale of the spectrum can expand and contract during the logging process like a spring fixed at one end. The M-factor adjusts the stretch of the spring while the A-factor adjusts where channel zero is fixed on the energy scale. In other words, this is a drift correction. The accuracy of this correction depends on how well the Atlas postprocessing was able to estimate the correct M and A values as a function of depth in the borehole. In any event, this processing step is performed just as Western Atlas

would perform it, so analyzing the success of this step contributes to the log quality analysis. The program writes the rechannelized spectra in the same format as the input spectral file. CALSPEC calls one user-defined function, RECHAN (to rechannelize the spectral data).

5. *Manual operations.* The analyst next works through the blueline, making a list of depth ranges over which to sum the spectral data. All depths must be rounded to the nearest whole foot and the bottom of one range should be separated by a foot or more from the top of the next range; these restrictions were imposed to simplify the programming but could be removed with minor effort. Typically the zones selected for summing have similar radioelement characteristics such as, say, a ^{137}Cs anomaly, or a zone with no artificial nuclides indicated.

6. *Run the program SUMSPEC.* This program sums spectral data over one or more specified depth ranges and writes output data files in the format required by subsequent processing steps (programs COMBSPEC, STRIPNAT, and ARTIFIT). The result is one output data file for each specified depth range. Each output data file contains a 256-channel spectrum summed over the depth range, along with supporting information such as nominal M and A values for the rechannelized spectrum, depth information, and sample time.

Before running the program, the analyst should check the format of the full spectral data against the input format required by SUMSPEC. He or she should also change the file names and paths specified in the program so they correspond to the existing disk files, and specify the number of depth ranges to sum over and the upper and lower depth limits for each depth range.

SUMSPEC calls one user-defined function, READSPC3 (to read spectral data from disk). The default condition is that output data files are automatically assigned names like 09451021.DAT; that file would contain data summed over the depth range of 945 ft to 1021 ft.

7. *Run the program COMBSPEC (optional).* This optional step in the processing combines data from two or more output files from SUMSPEC. This step might be performed, for instance, to combine all the barren zone data into one file. COMBSPEC does not call any user-defined functions. Before running this program, the analyst specifies file names and paths and specifies the number of input files to be read (each input file contains one spectrum summed over a specified depth range). The output file format is the same as the input file format so files created by COMBSPEC can be treated the same as those created by SUMSPEC.

8. *Manual operations.* At this stage, the spectra have been energy-calibrated, summed over specified depth ranges, and converted to counts per second. Also, the summed spectra from multiple depth ranges have been combined, if desired. In the next steps, the contributions of naturally-occurring gamma emitters are subtracted from one of these summed spectra to determine if artificial nuclides are present. This process is accomplished interactively by subtracting scaled spectral templates for potassium, uranium and thorium from the summed field spectrum. Progressive subtraction actually begins with the thorium family, followed by the uranium family, and finally ^{40}K . The process starts with the thorium family because the 2.614 MeV peak from ^{208}Tl is the highest-energy peak of any nuclide that is likely to be found in quantity at the NTS so it can be scaled by eye (referring to plots) without interference from other nuclides. Uranium is subtracted second because, after thorium, the uranium family has the highest energy peaks. Any *residual spectrum* remaining after the estimated spectral contributions of the three natural radioelement families are subtracted should be attributable to artificial nuclides plus noise resulting from counting statistics and errors that creep into the results as successive processing steps are performed.

Corresponding to each summed spectral file created by SUMSPEC, the user must manually create (using a text editor) a corresponding parameter file with the same name but a file extension of *.PAR. For example, if the summed data file is named 20552670.DAT (i.e., summed over the depth range from 2055 ft to 2670 ft) the corresponding parameter file would be named 20552670.PAR. The parameter file is used in subsequent processing steps to control, for example, the scaling of the spectral templates before they are subtracted from the summed field spectra.

Each parameter file contains values for the following parameters: TemplateScaleFactor, YAxisMax and YAxisMin, and FieldM and FieldA, as explained below.

- TemplateScaleFactor is a vector of 18 numbers. Each of the 18 numbers is a scale factor corresponding to one of 18 spectral templates provided by Western Atlas. The templates are stored in template files in the following order: (1) ^{40}K , (2) ^{238}U , (3) ^{232}Th , (4-6) ^{125}Sb , (7-9) ^{106}Ru , (10-12) ^{137}Cs , (13-15) ^{134}Cs , (16-18) ^{60}Co . Note that there are three templates for each artificial nuclide just as described in Table 3 above. These three templates (for example, templates 4-6 for ^{106}Ru) represent three different calibration environments: (a) the logging instrument in a simulated borehole in a sandstone block with a button calibration source located 3 in inside the borehole wall in a small hole drilled from the outside of the block, (b) as above but with a button calibration source located 1 in inside the borehole wall, and (c) the logging instrument hanging in air with the button source about 13 in from the pressure housing. Western atlas personnel routinely use the template made with the source 1 in inside the borehole wall (case b, above) to represent each artificial nuclide spectrum, concluding that these calibration spectra seem to represent the best fit to the field data.
- YAxisMax and YAxisMin are the scale factors for the ordinate of the residual spectrum plots, that is, the maximum and minimum values on the Y axis.
- FieldM and FieldA are additive correction factors used to adjust M and A if desired, for example, if the Western Atlas values appear to be incorrect. If no correction is needed, these are set to zero. More frequently, some fine-tuning of the energy calibration is necessary and these parameters are used to refine the fit between the spectral templates and the field spectrum. Increasing FieldA shifts the field spectrum toward lower energies without stretching or compressing it and, conversely, decreasing FieldA shifts the field spectrum toward higher energies. Similarly, increasing FieldM compresses the field spectrum on the energy scale while leaving the offset unchanged, while decreasing FieldM stretches the field spectrum to higher energies.

An example of a parameter file is given in Table 4. In this file, scale factors of 0.52, 0.145, and 0.215 are given for, respectively, the natural potassium, uranium, and thorium templates. This means, for example, that the thorium spectral template is multiplied by 0.215 and subtracted from the field spectrum to strip out the thorium contribution. Also, scale factors of 0.42 are given for all three geometries for the ^{137}Cs spectral template. In practice, only one of the geometries is likely to be used. Y axis maximum and minimum values are specified at 1 and -1, respectively, for the plots of the residual spectra. Finally, adjustments are specified for gain M (0.8) and offset A (-2.0) for the .

Table 4. Sample parameter file.

```

TemplateScaleFactor
0.52
0.145
0.215
0.0
0.0
0.0
0.0
0.0
0.0
0.0
0.042
0.042
0.042
0.0
0.0
0.0
0.0
0.0
0.0
0.0
YAxisMax for residual spectrum
1
YAxisMin for residual spectrum
-1
FieldM additive adjustment
0.8
FieldA additive adjustment
-2.0
    
```

9. *Run the program STRIPNAT.* This program backs out the natural spectral components interactively. This includes adjusting the M and A factors given in the summed field data files output by SUMSPEC or COMBSPEC. It also includes adjusting the first three values in TemplateScaleFactor, a vector of 18 multiplicative scale factors corresponding to the 18 spectral templates. The first 3 values in ScaleFactor correspond to K, U, and Th templates. The three spectral templates for the three natural nuclide families were developed using data from the API spectral gamma test pits, 8.5-inch diameter, uncased, and water-filled.

Before running STRIPNAT, the analyst creates a parameter file corresponding to the input spectral data file as described above. Also, he or she edits the source file STRIPNAT.M as follows:

1. Specify the borehole name
2. Specify the depth range or other file name such as 'clean' (for all clean zones)
3. Specify a graph title if a depth range is not used
4. Specify which spectral templates are to be used

Raw spectral templates for K, U, Th, and five artificial nuclides are read in from the template data file (generally AWSTEMP2.DAT). The templates are converted to counts/s, rechannelized if necessary to adjust gain and offset, and normalized to unit source strength (this latter feature requires source strength calculations for the calibration sources and was never fully implemented, nor was it needed for the qualitative data produced for the UGTA program).

Next, the summed field spectrum written by SUMSPEC or COMBSPEC is rechannelized and natural the K, U, and Th components (i.e., the scaled spectral templates) are subtracted interactively to produce a residual spectrum that is written to disk. STRIPNAT calls two user-defined functions, RECHAN (to rechannelize the spectral data) and READTEMP (to read the template data from disk). After removal of the natural spectral components, the resulting residual spectrum is plotted with each of the artificial nuclide spectral templates for reference, to help assess whether artificial nuclides are present. If the stripping has been done correctly, this residual spectrum should consist of the contribution of artificial gamma emitting nuclides, if any, plus noise of various sorts resulting from imperfections in the logging system and processing procedures.

10. Manual operations. As explained in the previous step, STRIPNAT plots the summed field spectrum along with the scaled spectral templates. In the next step, the analyst carefully examines these plots to assess the goodness-of-fit between the template and the field spectrum. Then, the gain, offset, and template scale factors in the parameter file are adjusted to optimize the fit between the field spectrum and the scaled templates. This interactive, iterative procedure (steps 8, 9, and 10) is repeated until the stripping of the natural spectral components meets with the approval of the analyst.

11. Run the program ARTIFIT. This program is very similar to STRIPNAT except, rather than scaling and fitting the spectral templates for the three natural gamma emitters to a summed field spectrum, ARTIFIT is used to fit spectral templates for the five artificial gamma emitters to a residual spectrum produced by the stripping process carried out by STRIPNAT. Thus, ARTIFIT is used to help estimate the concentrations of artificial nuclides that may be present, if any. If it appears that no artificial nuclides are present, it is generally not necessary to run this program. ARTIFIT calls two user-defined functions, RECHAN (to rechannelize the spectral data) and READTEMP (to read the template data from disk).

ARTIFIT reads the same summed data files read by STRIPNAT (such as the example 03450921.DAT, described above) as well as the same parameter file (e.g. 03450921.PAR). The final 15 of the 18 values in the vector ScaleFactor are the multiplicative scale factors for the 15 artificial nuclide templates, three each for Sb-126, Ru-106, Cs-137, Cs-134, Co-60, in that order, as shown in Table 3. The three templates in each group of three are for (1) the tool hanging in air with the source about 13 inches away, (2) in an open 12-inch borehole with the source 1 inch into the (sandstone) formation, and (3) in an open 12-inch borehole with the source 3 inches into the formation. All are background subtracted.

Before running ARTIFIT, the analyst edits the parameter file corresponding to the input spectral data file as described above. Also, he or she edits the source file ARTIFIT.M as follows:

1. Specify the borehole name
2. Specify the depth range or other file name such as 'clean' (for all clean zones)
3. Specify a graph title if a depth range is not used
4. Specify which spectral templates are to be used

12. Manual operations. As explained in the previous step, ARTIFIT plots the residual spectrum along with the scaled spectral templates corresponding to the five artificial gamma emitters. In the next step, the analyst carefully examines these plots to assess the goodness-of-fit between the templates and the residual spectrum. Then, the gain, offset, and template scale factors in the parameter file are adjusted to optimize this fit and this interactive, iterative procedure (steps 11 and

12) is repeated until the analyst has adequately assessed the artificial nuclide components of the spectral gamma-ray log data.

User-defined functions

The programs used in the routine processing of AWS spectral gamma-ray data call several functions, described here. Listings for the functions are given in Appendix B where the parameters in the function calls are described in comment statements.

Function name: **RECHAN**

Used by: CALSPEC, STRIPNAT, ARTIFIT

Purpose: Rechannelize full-spectral data.

Function call: [RechEnergy,RechSpectrum] = rechan(Spectrum,M,A,RechM,RechA)

Function: **READSPC3**

Used by: SUMSPEC

Purpose: Read the spectral data written by CALSPEC.

Function call: [NormalizedSpectrum,TotalTime,LastDepthRead,NDepthsSpecified, ...
NDepthsActual,RawM,RawA,RechM,RechA] = readspc3(UpperDepth,
LowerDepth,DataFileID,FirstRead);

Function: **READTEMP**

Used by: STRIPNAT, ARTIFIT

Purpose: Read the AWS spectral templates.

Function call: [AtomicWeight,Casing,BHDia,BHFluid,SourcePosition,Cal1,Cal2,Spec,...
AccumulationTime] = readtemp(TemplateFileName);

Special-purpose programs

In addition to the programs used in routine processing, described above, many special-purpose programs were developed for specific limited purposes. Several of these are useful enough in general to be included here.

REMOVBKG: Performs a rough background subtraction on Western Atlas spectral templates using an interactive procedure. First, the templates are plotted along with a synthetic background spectrum and a background-corrected curve. The background-subtracted templates are written to disk. The user adjusts the parameters for each of the synthetic background spectra until an acceptable fit is obtained. This is used to adjust the background components of two spectra to be more similar to allow them to be compared more readily. Program REMOVBKG calls functions READTEMP and RECHAN, described above.

LOWERRES: Reduces the energy resolution of the spectrum using an empirical, energy-dependent filter. This is used to adjust the energy resolution of an accumulated spectrum so it is similar to that of another, lower-resolution accumulated spectrum, so they may be compared more readily. Program LOWERRES calls function RECHAN, described above.

TEMPLOT1: Plots the 18 spectral templates supplied by Western Atlas, one per page. Program TEMPLOT1 calls functions READTEMP and RECHAN, described above.

TEMPLOT3: Plots the 18 spectral templates supplied by Western Atlas 3 to a page, with the corresponding SYNTH spectrum when available. SYNTH is a program developed by Pacific Northwest National Lab to generate synthetic gamma-ray spectra for specified nuclides. Program TEMPLOT3 calls functions READTEMP and RECHAN, described above.

Real-world examples

For a better understanding of how the data analysis procedure described in this report is used in practice, refer to any of the five data analysis reports produced in 1997 for the UGTA program.¹⁻⁵ For convenience, one of these data analysis reports, for borehole ER-20-6 #1,³ is reproduced in Appendix C.

References

- {1} J. G. Conaway, "Spectral gamma-ray log data analysis for NTS borehole ER-20-5 #1," Los Alamos Report LA-UR 97-2042 (1997).
- {2} J. G. Conaway, "Spectral gamma-ray log data analysis for NTS borehole ER-20-5 #3," Los Alamos Report LA-UR 97-3584 (1997).
- {3} J. G. Conaway, "Spectral gamma-ray log data analysis for NTS borehole ER-20-6 #1," Los Alamos Report LA-UR 97-1087 (1997).
- {4} J. G. Conaway, "Spectral gamma-ray log data analysis for NTS borehole ER-20-6 #2," Los Alamos Report LA-UR 97-1088 (1997).
- {5} J. G. Conaway, "Spectral gamma-ray log data analysis for NTS borehole ER-20-6 #3," Los Alamos Report LA-UR 97-1457 (1997).
- {6} J.G. Conaway, "Identification of artificial gamma-emitting nuclides using a scintillation-based gamma-ray spectral logging system," *Fourth Annual Symposium on Borehole Geophysics for Geotechnical and Groundwater Applications*, Minerals and Geotechnical Logging Society, Toronto, August 26-30, 1991.

APPENDIX A

PROGRAM FLOW CHARTS

This appendix contains flow charts of the standard programs described in the main body of this report as well as a flow chart describing the standard processing procedure graphically. The symbol key for the flow charts is given at the bottom of this page. The flow charts are given in the following order:

1. Overall processing flow chart.
2. Flow charts of the standard programs for processing AWS spectral gamma-ray borehole data for the UGTA program.
 - A. CALSPEC
 - B. SUMSPEC
 - C. COMBSPEC
 - D. STRIPNAT
 - E. ARTIFIT

Symbol key for the flow charts.

OVERALL DATA ANALYSIS PROCEDURE FLOW CHART

Figure A1. Flow chart showing the overall data analysis procedure for routine spectral gamma-ray log analysis in the UGTA program. Flow charts are given separately for each of the five MATLAB programs represented here: CALSPEC, SUMSPEC, COMBSPEC, STRIPNAT, AND ARTIFIT.

Program CALSPEC

Figure A2. Flow chart showing procedure used in CALSPEC.M.

Program SUMSPEC

Figure A3. Flow chart showing procedure used in SUMSPEC.M.

Figure A4. Flow chart showing procedure used in COMBSPEC.

Figure A5. Flow chart showing data processing procedure used in STRIPNAT.

Figure A6. Flow chart showing data processing procedure used in ARTIFIT.