

GJO-HGLP 1.6.3
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Hanford Geophysical Logging Project
Data Analysis Manual

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Prepared for
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1.0 Overview

In 1995, the U.S. Department of Energy Grand Junction Office (DOE-GJO) was requested by the DOE Richland Operations Office (DOE-RL) to perform a baseline characterization of the vadose zone around the single-shell tanks (SSTs) at the Hanford Site. The intent of this characterization project was to determine the nature and extent of gamma-ray-emitting radionuclide contamination in the vadose zone, to identify contamination sources where possible, and to develop a baseline of the contamination distribution that will permit future data comparisons. This task was accomplished using high-resolution spectral gamma-ray geophysical methods.

Baseline characterization of the Hanford SSTs was completed in 2000. The project has since been extended to perform a baseline characterization of the vadose zone in the vicinity of other waste disposal sites in the Hanford 200 East and 200 West Areas. Numerous liquid and solid waste disposal sites are located in close proximity to the SST tank farms. Although the bulk of the radioactivity was disposed to the SSTs, liquid waste sites are known to have received significant radioactivity as well as substantial liquid volumes. Given the close proximity of the various sites, it is likely that contaminant plumes have intermingled in the vadose zone, and examples are known where relatively low-level wastes discharged at one site have migrated laterally and mobilized contaminants associated with discharges to another waste site. The end result is that the nature and distribution of vadose zone contamination in the Hanford 200 West and 200 East Areas are very complex.

In general terms, high-resolution gamma-ray spectra are collected by logging existing vadose zone boreholes. Two spectral gamma logging systems (SGLs), manufactured by Greenspan, Inc., are used to record spectra at discrete depth increments in the boreholes. The radionuclide sources of the gamma rays are determined from the energy of the gamma rays. The concentrations of source radionuclides are determined by applying calibration constants and correction factors to the net count rates for each of the radionuclides identified. Data are then plotted as the concentrations of various radionuclides at specific depths.

In addition, the U.S. Department of Energy Office of River Protection (DOE-ORP) has requested DOE-GJO to develop and implement a monitoring program in selected boreholes in the single-shell tank farms.

The Radionuclide Assessment System (RAS) was developed for monitoring purposes. This logging system utilizes a series of three sodium iodide (NaI) detectors for routine monitoring purposes.

This manual describes the flow of data from collection through analysis and presentation and provides an overview of the data analysis process, descriptions of individual software packages, and requirements for data handling and archiving. This manual is intended for use as both a user's manual and reference manual for the data analysis system in general for both the Hanford 200 Areas Spectral Gamma Baseline Characterization Project (DOE-RL) and the Hanford Tank Farms Vadose Zone Monitoring Project (DOE-ORP). Whenever possible, information necessary for data analysis is presented in tables to facilitate ready reference during analysis.

The analyst should be familiar with and comfortable in the use of Microsoft *Windows NT 4.0* or *Windows 95/98*. Other general-purpose software, such as *Word*, *Excel*, *SigmaPlot*, *Adobe Acrobat*, and *PKZip* are used to manipulate data. Special-purpose software such as *Aptec PCMC/WIN* and *OSQ/Supervisor* are used to process gamma energy spectra. A three-dimensional visualization program called *Environmental Visualization Systems (EVS)* is used to extrapolate borehole data and provide visualizations. A limited amount of in-house software is used, primarily to convert and parse data. The analyst should be familiar with the operation of these programs.

2.0 Processing Flow of Log Data

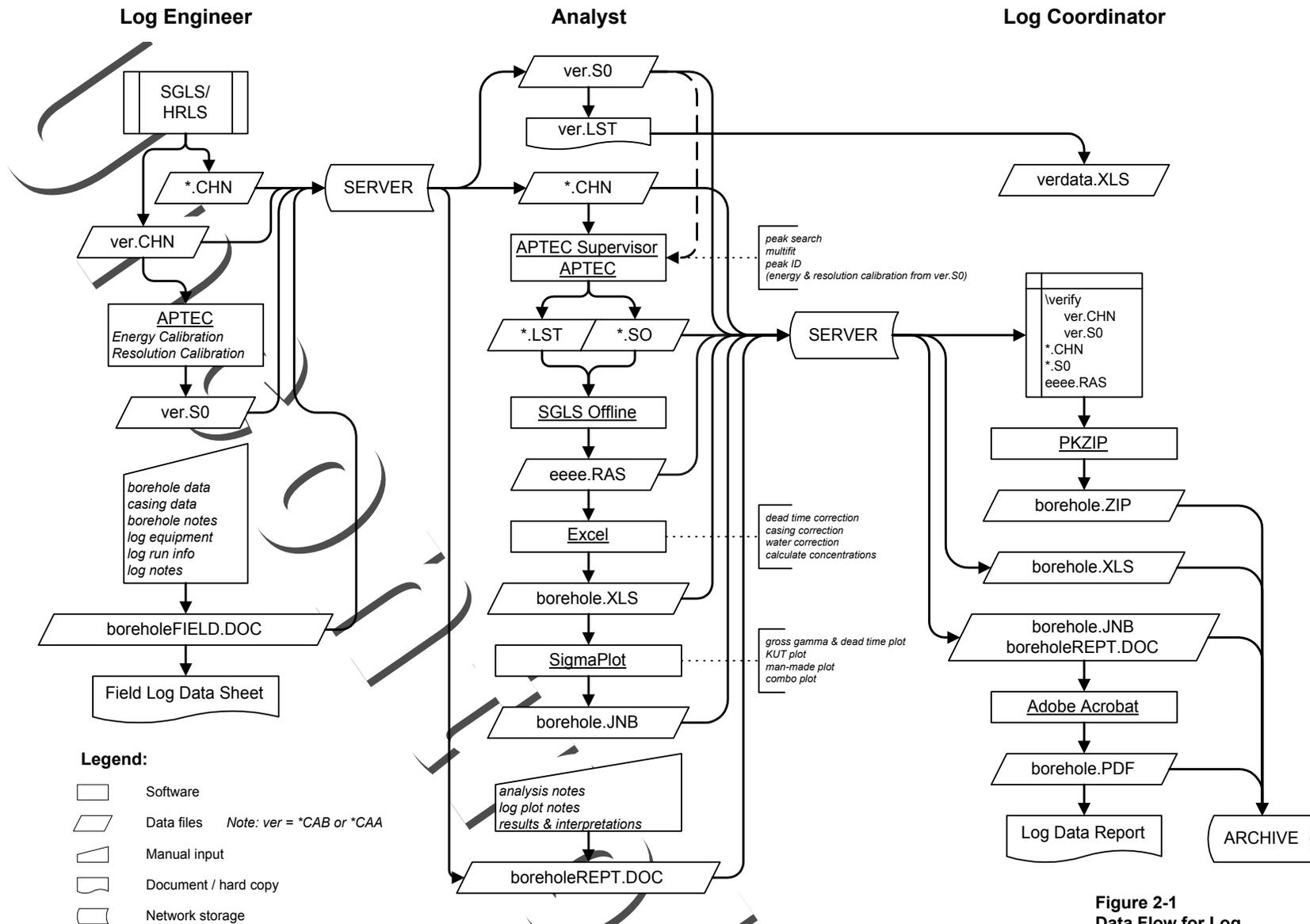
Current logging capabilities include three types of logging systems: the spectral gamma logging system (SGLS), the high rate logging system, (HRLS), and the neutron moisture logging system (NMLS). An additional system, the radionuclide assessment system (RAS), has been developed specifically for monitoring purposes in the Hanford single-shell tank farms.

The data flow described in the following sections contains several provisions to safeguard data integrity. Field data are loaded onto a separate subdirectory within the server. When log data are processed, the field data are copied to the local hard drive, and processed data are then transferred back to the server. Raw spectra are saved as *.CHN files, while processed spectra are saved as *.S0 files.

2.1 SGLS and HRLS Data Processing

Figure 2-1 illustrates the data flow process for SGLS data processing and analysis. HRLS data are handled in a similar manner. HRLS and SGLS data consist of individual spectral measurements made at discrete depth intervals, typically 0.5 or 1.0 feet (ft). These spectra consist of individual gamma counts sorted by increasing energy into 4096 channels. Fine-gain adjustments may be made during logging to assure consistency in peak/channel alignment. Gamma spectra are saved as individual files for each depth increment. Each file contains header information including borehole identification, depth, start time, real time, and live time. Raw (unprocessed) log data are saved as *.CHN files. These are binary files formatted according to the *Ortec* specification for multichannel spectra. The specific format for these files is presented on pages 43 and 44 of the CASASII (*Computer Automated Spectral Acquisition System II*) manual (Greenspan). During logging, the logging engineer completes a Log Data Sheet (located on the field laptop computer) that records information including general borehole data, casing information, borehole notes, log equipment information, log run information and log notes using Microsoft *Word*. The logging engineer typically will also process and evaluate the pre-run verification spectra and compare peak intensities and resolution (in terms of full width at half maximum, or FWHM) for selected peaks to previously established verification criteria.

For the purposes of this manual, lower case italics in the following spectrum name indicate alphanumeric codes with variable characters. Individual spectra have a file name of the form *vsrrrnnn.CHN*. The first character, *v*, indicates the logging unit, and the second character, *s*, indicates the sonde with which the log was collected. Each logging unit and sonde are designated by unique characters. Currently (March 2002) two logging units (designated A and B) and five sondes are available: three SGLSs (A, B, D), one HRLS (C), and one NMLS (F). Codes for sonde-logging unit combinations are shown in Table 2-1.



**Figure 2-1
Data Flow for Log
Processing & Analysis**

Table 2-1. Calibrated Sonde-Logging Unit Combinations (October 2002)

Designation			Serial No.	Logging Unit		
New	Old			1 Gamma 1	2 Gamma 2	3 RLS
A	Y1A	SGLS (spare)	34TP20893A		X (Sept. 02) ¹	
B	Y2B	SGLS	36TP21095A		X (Sept. 02)	
C	Y1C	HRLS	39A314	X (Feb. 01)		
D	Y2A	SGLS	34TP11019B	X (Sept. 02)		
E	RLS-1	70% HPGe	34TP40587A			X (Oct. 02)
F		NMLS	H380932510		X (Sept. 02)	

¹ Last calibration date

The code *rrr* designates a sequential log run number, which is incremented for each log run. The *nnn* code is a sequential number starting with 000 and incremented for each successive spectrum.

The above files are saved with the Log Data Sheet (saved as *borehole_FIELD.DOC*) (Figure 2-2) on the hard disk of the field laptop computer. At the end of each day, the files are copied onto a zip disk. After a borehole log is completed, the data files are brought into the office by the project coordinator and transferred from the zip disk onto disk storage on the office server, with separate subdirectories for each borehole. In addition to the files stored on the server, a hard-copy report file contains supplemental information and a printed copy of the *borehole_FIELD.DOC* file and any verification spectra listings. A single *borehole_FIELD.DOC* file may contain notes from several days of logging operations. The code *borehole* is a unique identifier for each borehole. For complex logging events, multiple *.DOC files may summarize field data.

Log data processing begins when the analyst copies the field data from the network hard drive to a local hard drive. A variety of additional files are generated during log processing. Table 2-2 describes files for a typical borehole log dataset. For each *.CHN file, *.S0 and *.LST files are generated. *.S0 files are binary files formatted according to the *Aptec* specification for spectral data. Energy and resolution calibrations and data for regions of interest are embedded in the file. A detailed description of the *Aptec* file format is provided in pages 75 to 85 of the *Aptec PC/MCA/WIN Installation and Operations Manual*. For the purpose of this project, all processed spectra are saved as *.S0 files.

*.LST are text files produced by *Aptec* that contain results of the peak search, multifit, and peak identification for each spectra. Several choices for content and format are provided. However, the *SGLSoffline* program used to read and parse these files is set up

to read the data in a specific format. Therefore, standard *.LST file formats as indicated in the respective tables must be used.

For each data point, *.CHN files represent the raw measurement data, and the *.S0 and *.LST files represent the output of the spectral processing step. *.RAS files are text files

S.M. Stoller Corp. BOREHOLE DATA SHEET	Borehole	
	Date	

Logging Equipment Information:

Log System:	Type:	Serial No.:
Logging Procedure:		
Calibration Date:	Calibration Reference:	

Log Run Information:

Date				
Start Depth (ft)				
Finish Depth (ft)				
Count Time (sec)				
Live/Real				
Shield				
MSA Interval				
Log Speed				
Pre-Run Verification				
Start File				
Finish File				
Post-Run Verification				
Depth Return Error (in.)				
Comments:				

Logging Operation Notes:

Data File Location:

--

Signature:	Date:
-------------------	--------------

Figure 2-2. Sample Log Data Sheet

Table 2-2. Log Data File Descriptions

	File Name	Format	Contents
Field Data Files	<i>vsrrrrnnn</i> .CHN	Ortec	Individual gamma spectra (counts vs. channel) stored as binary files formatted according to the <i>Ortec</i> specification.
	<i>vsrrrr</i> CAB.CHN <i>vsrrrr</i> CAA.CHN	Ortec	Pre-run and post-run verification spectra.
	<i>vsrrrr</i> CAB.S0 <i>vsrrrr</i> CAA.S0	Aptec	Processed verification spectra.
	<i>vsrrrr</i> CAB.LST <i>vsrrrr</i> CAA.LST	text	Verification spectra listing files.
	<i>borehole</i> _FIELD.DOC	Word	Field data report. Borehole data, casing data, borehole notes, log equipment notes, log run information, and logging notes.
	Office Data Files	*.JOB	Aptec Supervisor
<i>vsrrrrnnn</i> .S0		Aptec	Processed log spectra.
<i>vsrrrrnnn</i> .LST		text	Log spectra listing files.
<i>eeee</i> .RAS		text (fixed length)	Data files generated by <i>SGLSoffline</i> . Net counts, error, MDA, and % dead time as a function of depth for peak at energy <i>eeee</i> (keV).
grosscnts.RAS		text (fixed length)	Data file generated by <i>SGLSoffline</i> . Total counts and % dead time as a function of depth.
NMLS.CSV		text (comma delimited)	Data file generated by <i>Supervisor</i> during analysis of NMLS data. Total neutron counts as a function of depth.
<i>borehole</i> .XLS		Excel	<i>Excel</i> workbook for concentration (activity) calculations. Includes worksheets for I(E), dead time correction, casing and water corrections, as well as individual worksheets for each energy peak. May also include preliminary plots.
<i>borehole</i> .JNB		SigmaPlot	<i>SigmaPlot</i> workbook used to generate log plots. Includes concentration, concentration error, and MDL as a function of depth.
<i>borehole</i> .DOC		Word	Log Data Report. Includes borehole data, casing data, borehole notes, log equipment notes, log run information, and logging notes from the field data file, as well as analysis notes, log plot notes, and results and interpretations.
<i>borehole</i> .PDF	Adobe Acrobat	Final electronic deliverable created by Log Coordinator. Includes contents of <i>borehole</i> .DOC and plots from <i>borehole</i> .JNB in Adobe portable document format (read only).	

Notes:

- vsrrrrnnn* = unique spectra file identifier
v = logging unit identifier (*A* = Gamma 1, *B* = Gamma 2)
s = sonde identifier (*A,B,D* = *SGLS*, *C*=*HRLS*, *F*=*NMLS*)
rrr = run number
nnn = spectrum number
- CAB and CAA indicate pre-run and post-run verification measurements
- borehole* = unique identifier for a specific borehole (e.g. *E33-286* or *C3102*)
- eeee* = energy level, nearest keV

produced by the *SGLSoffline* program from the *.LST and *.S0 files for a given borehole. One *.RAS file is generated for each energy peak identified in any of the *.LST files, (i.e., one for each isotope identified by the *Aptec* software). *.RAS files have a filename of the form *eeee*.RAS, where *eeee* designates the energy level of a specific peak. For example 0662.RAS contains data for the 662-keV peak. The *.RAS file will contain one line for each depth at which the peak was encountered. A GROSSCNTS.RAS file contains gross (total) counts as a function of depth. Data fields in the *.RAS file are fixed length. Columns in an *eeee*.RAS file are:

- depth measurement depth (ft)
- deadtime percent dead time
- cps net count rate for peak
- cpsUnc uncertainty in net count rate (in percent)
- mda minimum detectable activity
- flag flag indicating type of value
- filename spectrum file name

An *Excel* workbook (*borehole.XLS*) is used to calculate concentrations from net count rates in the *.RAS files. Each *.XLS file contains worksheets for the calibration function and correction functions, as well as individual worksheets for each energy peak used for analysis. The *.XLS file also includes a *description* worksheet that defines all variables and parameters used in the calculation process. Concentration data from the *borehole.XLS* file are transferred to a *SigmaPlot 8.0* file (*borehole.JNB*). *SigmaPlot* files are organized in a workbook fashion, with one or more sections each containing a data worksheet and one or more graph pages. Each graph page may contain several graphs, with multiple plots on each graph.

Notes, assumptions, observations, and interpretations related to the analysis process are stored in *borehole.DOC*, a Microsoft *Word* file. When the processing is complete, *borehole.DOC* and graph pages from *borehole.JNB* are printed to an Adobe *Acrobat* file, *borehole.PDF*, which constitutes the electronic data deliverable.

Given below are instructions for data flow during processing and analysis of SGLS and HRLS log data. For specific information on each step, refer to the appropriate section of this procedure.

1. Locate the directory for the correct borehole. The typical file structure for field data is given in Figure 2-3. Check that all data are present and copy the files to the local hard disk for analysis. When appropriate, additional subdirectories may be added to segregate different log events or individual runs. Read through the hard copy report file for the borehole and note any special conditions or additional data that may affect either analysis or interpretation.
2. Review any pre-run and post-run verification spectra that were processed in the field, and process any remaining verification spectra. (Processing of verification spectra is discussed in Section 3.) The processed files should be saved as *.S0

under the \VERIFY subdirectory. Print a copy of the spectra listing for each verification spectrum and include it in the hard copy file. Highlight the appropriate peak intensities and FWHM values and compare them to the verification criteria.

```
\PROJECT DATA\200AREAS\ LOGDATA\200EAST\borehole
[example]

...   \borehole
      borehole_FIELD.DOC
      \SGLS
          vsrrrnnn.CHN
          vsrrrCAB.CHN
          vsrrrCAA.CHN
          vsrrrCAB.S0
          vsrrrCAA.S0
      \HRLS
          vsrrrnnn.CHN
          vsrrrCAB.CHN
          vsrrrCAA.CHN
          vsrrrCAB.S0
          vsrrrCAA.S0
      \NMLS
          vsrrrnnn.CHN
          vsrrrCAB.CHN
          vsrrrCAA.CHN
```

Figure 2-3. Field Data Server Directory Structure

3. Set up *Aptec Supervisor* for batch processing of the log data. (Batch processing with *Aptec Supervisor* is discussed in Section 4.) After all parameters have been set, save the file (*.JOB) in the same directory as the *.CHN files and execute the batch run. This will generate a series of *.S0 and *.LST files, which should be stored in the same directory as the *.CHN files.
4. Review individual spectra and make changes as necessary. After all spectra have been reviewed, run *LISTEM.BAT* to generate *.LST files from the final *.S0 files.
5. Run *SGLSoffline* to consolidate the log data. *SGLSoffline* reads the individual *.LST and *.S0 files and generates a separate file for each gamma energy peak identified in the individual spectra. These files are of the form *eeee.RAS*, where *eeee* indicates the energy level. For example 0662.RAS is the file for data associated with the ¹³⁷Cs peak at 661.66 keV. These files are saved in the same directory as the corresponding *.CHN and *.S0 files.

6. Select the appropriate *.RAS files and import them into the *Excel* workbook for the correct logging system and calibration date. Immediately save the *Excel* file as *borehole.XLS*.
7. After completing data processing with the *borehole.XLS* file in *Excel*, transfer the log data to a *SigmaPlot* workbook and immediately save it as *borehole.JNB*.
8. Complete log plotting in *SigmaPlot*. Using a previous *borehole.DOC* file as a template, open the *borehole_FIELD.DOC* file in *Word* and copy relevant data to the template, making corrections and additions as necessary. Add analysis notes, log plot notes, and results and interpretations. Save the new file (with the new borehole name) as *borehole.DOC*. Print hard copies of *borehole.DOC* and all plots. Include these in the hard copy folder for review.
9. After review by the technical lead has been completed, make appropriate changes or corrections and ensure that the latest files for the borehole are properly organized in the server field data directory. Figure 2-4 shows a typical directory structure for processed log data. The *.LST files for log spectra can be deleted, because all data are contained in the *.S0 file.
10. Pass the hard copy file to the log coordinator. The log coordinator will enter verification data into the VERDATA.XLS workbook. Output from *borehole.DOC* and plots from *borehole.JNB* will be combined into a Log Data Report using Adobe Acrobat and saved as *borehole.PDF*.
11. The log coordinator will compress all *.CHN, *.JOB, *.S0, and *.RAS files, and *borehole_FIELD.DOC* into a file *borehole.ZIP*, using *PKZip*. The files *borehole.PDF*, *borehole.DOC*, *borehole.JNB*, *borehole.XLS*, and *borehole.ZIP* constitute the log data package. Borehole data will be removed from the server when the Waste Site Summary Report including that data is issued. Borehole data for a particular waste site will be archived on a CD-ROM included with individual Waste Site Summary Reports. Additional copies of the archive files will be included on CD-ROM (in order of completion) and stored in the office with a duplicate copy stored in another location.

2.2 NMLS Data Processing

Analysis of neutron moisture log data does not require the same level of processing as SGLS and HRLS data, and the data flow is correspondingly simpler. Neutron log data consist of *.CHN files organized in much the same way as SGLS or HRLS data. Pre-run and post-run verification spectra are also stored as *CAB.CHN and *CAA.CHN files. Neutron log information and log notes pertinent to the neutron log generally are recorded by the logging engineer in the *borehole_FIELD.DOC* file discussed above. Although the data are saved as spectra (*.CHN files) by the logging software, only the total counts in each spectra are of interest. Because NMLS data typically are collected concurrently with SGLS and/or HRLS data in the same borehole, the data flow generally follows that

\PROJECT DATA\200AREAS\ LOGDATA\200EAST\borehole
[example]

```
...  \borehole
      borehole_FIELD.DOC
      borehole.DOC
      borehole.XLS
      borehole.JNB
      \SGLS
          vsrrrnnn.CHN
          vsrrrnnn.S0
          vsrrrnnn.LST
          eeee.RAS
          grosscnts.RAS
          *.JOB
          \VERIFY
              vsrrrCAB.CHN
              vsrrrCAA.CHN
              vsrrrCAB.S0
              vsrrrCAA.S0
              vsrrrCAB.LST
              vsrrrCAA.LST

      \HRLS
          vsrrrnnn.CHN
          vsrrrnnn.S0
          vsrrrnnn.LST
          eeee.RAS
          grosscnts.RAS
          *.JOB
          \VERIFY
              vsrrrCAB.CHN
              vsrrrCAA.CHN
              vsrrrCAB.S0
              vsrrrCAA.S0

      \NMLS
          vsrrrnnn.CHN
          grosscnts.CSV
          *.JOB
          \VERIFY
              vsrrrCAB.CHN
              vsrrrCAA.CHN
```

Figure 2-4. Processed Log Data Server Directory Structure

of the SGLS as discussed above, and the data are incorporated into the *borehole.XLS* and *borehole.JNB* files.

2.3 RAS Data Processing

In contrast to conventional logging practice, log data processing for the RAS is not typically performed in the field. When rapid data reporting is necessary, it may be possible to generate a preliminary total gamma log and neutron logs within a short time after data collection, but detailed identification and quantification of specific radionuclides require extensive data processing. The RAS logging software generates a file of gross counts in each of eight energy “windows” as a function of depth. Although this file could be plotted in the field, the main purpose of the monitoring program is to detect changes between successive log runs, and this function is best performed in the office.

The RAS collects 256-channel spectra from the NaI(Tl) detectors used for monitoring. These are stored as *.CHN files. In general, there is no need to examine individual spectra. The RAS logging program also generates a data file with count rates for each of eight energy “windows” as a function of depth. RAS data are processed independently of SGLS data, although frequently comparisons are made between data collected from each system. RAS data are stored and processed in *Excel* workbooks. Each workbook contains the data for one borehole, including the SGLS data. The *.CSV file generated by the logging program is opened directly by *Excel* and the data are transferred to a new worksheet in the correct workbook. Plots are generated to compare successive log runs. After the data have been loaded in the spreadsheet, both the *.CSV file and all *.CHN files can be compressed with *PKZip* for archival.

2.4 Other Data Processing

RLS, gross gamma, or other previous log data may be evaluated for comparison to SGLS and HRLS data. When specific radionuclides are involved, it may be necessary to perform decay calculations so that the data can be compared on a common date. It may also be necessary to make depth adjustments or to recalculate concentrations. These calculations typically will be performed in a supplemental *Excel* workbook with the results transferred to the *SigmaPlot* file for plotting and comparison.

3.0. Verification Data Processing and Evaluation

Field verification spectra are recorded at the beginning and end of each logging day. These spectra are recorded in portable field verifiers, in which the detector response is well known. The verification spectra provide a means to assess long-term logging system performance and stability, as well as the continuing energy and resolution calibrations necessary for spectral analysis. Verification criteria are calculated for each logging unit/sonde combination from statistical analysis of verification measurements made during calibration measurements, as well as on-going logging activities. Currently available logging systems are listed on Table 2-1. Memoranda listing verification criteria for specific logging systems periodically will be issued by the project technical lead.

3.1 Development of Verification Criteria

Each unique combination of sonde and logging unit has a specific set of verification criteria based on one or more parameters measured by that system. These values are tracked in an *Excel* spreadsheet, which allows them to be plotted as a function of time. The mean (average) and standard deviation are also calculated for each parameter.

Verification criteria are stated in terms of upper and lower control limits. These are defined as the “3-sigma” limits, which should encompass more than 99% of the data, assuming the measurements are normally distributed. The upper and lower control limits are calculated for each verification parameter as follows:

$$UCL = \bar{X} + 3s$$

$$LCL = \bar{X} - 3s$$

Where \bar{X} is the average (mean) value and s is the (sample) standard deviation. During annual calibration, sets of verification measurements are made at the beginning and end of the calibration. Verification criteria are re-calculated after calibration. However, experience has shown that the logging systems tend to function differently over time, perhaps as a result of the rigors of the logging environment. Therefore, the control limits are calculated from a wider dataset that includes recent pre-run and post-run verification measurements. From time to time, verification criteria may be re-calculated by the technical lead.

Failure to meet verification criteria does not necessarily imply that the logging system is not functioning correctly. External radiation, ambient conditions, and the field environment associated with logging operations all affect system performance. When one or more verification parameters fall outside the control limits, the analyst should carefully examine individual spectra and overall system response. Verification measurements that fall outside the control limits may be provisionally accepted if the analyst can demonstrate that the system is functioning correctly. Note that there are no adjustments that can be made to improve system performance without compromising system calibration. Any adjustments made to a logging sonde to improve or restore performance will require recalibration for all logging systems using that sonde. Likewise, any adjustments made to the data collection equipment in a logging unit will require recalibration for all systems using that logging unit. The requirement for

recalibration may be waived when repeated verification measurements show no statistically significant difference from similar measurements collected before the modification.

3.2 SGLS Verification

When an SGLS is engaged in routine operations, field verification spectra are acquired with a *KUTh Field Verifier* (Amersham part number 188074). The verifier consists of a potassium-uranium-thorium source mounted in a hollow cylinder, which surrounds the sonde in the vicinity of the detector. Natural uranium- and thorium-bearing minerals were used to construct the verifier, such that the decay series are in secular equilibrium. Each verification spectrum thus has a number of prominent and stable full-energy peaks associated with various naturally occurring gamma-emitting radionuclides. A count time of 1,000 seconds typically is used for verification measurements to assure well-developed peaks. Figure 3-1 illustrates a typical SGLS verification spectrum on which the more prominent peaks have been labeled.

3.2.1 Processing SGLS Verification Spectra

Raw spectra are recorded in *Ortec* format as .CHN files. These spectra are processed individually using *Aptec* software to establish energy and resolution calibration, and to evaluate selected gamma peaks. Logging system performance evaluation is based on net counts (intensity) and full width at half maximum (FWHM) for the 609.3-keV gamma ray of ^{214}Bi (^{238}U decay product), the 1460.8-keV gamma ray of ^{40}K , and the 2614.5-keV gamma ray of ^{208}Tl (^{232}Th decay product). Consistent with conventional control chart practices (Taylor 1987), the intensities and FWHM are compared to acceptance tolerances derived from statistical analyses of peak intensities and FWHM from many previously recorded verification spectra. In general, pre-run verification spectra are processed in the field while logging is underway. Post-run verification spectra are later processed by the logging engineer or the data analyst. In either case, processed verification spectra are saved in *Aptec* (*.S0) format, which embeds the energy and resolution calibration developed during processing. Processing of SGLS verification spectra follows the basic steps outlined below. Specific details of the spectrum analysis process are discussed in Appendix B, and Appendix C provides a user guide for the *Aptec* software.

1. Set Up Analysis Parameters. Load the verification spectra (*.CHN) into *Aptec PCMCA/Win* software. Analysis parameters for SGLS verification spectra are provided in Table 3-1. These parameters can be entered in one of two ways. The first is to use *Edit/Load Header Information* to load the analysis setup from a previously analyzed spectrum (*.S0). After a spectrum is selected, this option displays a menu box with a number of check boxes selecting various components and parameters that can be imported. Ensure that all boxes are unchecked, except for "Analysis Setup." Analysis parameters can also be entered manually by using *Analyze/Setup* to configure *ROI Properties, Peak Search, Multifit, and Identification*. *Aptec* also allows user defaults to be saved; these parameters can be recalled by *Analyze/Setup/Analyze Defaults*.
2. Perform Peak Search. Use *Analyze/Peak Search* to locate spectral peaks. Specific details of the peak search process are discussed in the *Aptec* manual and in Appendix B. A key parameter in *Peak Search* is the "Max Peak Error." This defines the maximum net count

Table 3-1. Aptec Parameters for Processing SGLS Verification Spectra

Parameter	Recommended Value				
ROI Properties					
ROI Bkgnd Line	Least-squares fit, deg 3				
Use Method 2	X (yes)				
Centroid Calculated	Between Net Half Max				
Centroid Weighing	Net*abs(Net)*Chan				
Confidence	MDA Sigma = 1.645 Error Sigma = 2				
FWHM & FWTM Cal	Not used				
ROI Bkgnd End Points	10 End Channels (both sides)				
Peak Search					
Channel Range	150-4095				
Max Peak Error	50%				
Smooth Before Fitting	Do not check any boxes				
Energy Calibration					
Calibration Points	See below				
Max Degree	3				
Multifit					
Spectrum Type	HPGe/GeLi				
Optimize Centroid Search for	Separated Overlaps				
Peaks to be Fitted	Multiplets & Singlets Sigma = 1.645				
Fit Parameters	Fit with Peak Width: Fixed Fit with Background: Fixed				
Accuracy	Maximum Iterations = 20-40 Maximum Overlaps = 4-5 Percent Change = 0.25 Minimum Reduced Chi Square = 0.75				
Resolution Calibration					
	<i>Performed by MultiFit</i>				
Peak Identification					
Library	KUT.LIB				
Match ROI Centroid	Tolerance 3-4 keV				
Half Life limit	Not used				
Fraction Limit	25%				
Create "Force MDA"	no				
ROI Identification	Identify all ROIs				
Spectrum Listing					
Include	Header, Activities with FWHM				
Sort Isotopes	Alphabetically				
Report Errors As	Percentage ¹				
Save Listing File	ANSI (Windows)				
Recommended Energy Calibration Points					
	Radionuclide	Energy		Radionuclide	Energy
1	Ra-226 (U-238)	186.10	9	Ac-228 (Th-232)	911.21
2	Pb-212 (Th-232)	238.63	10	Ac-228 (Th-232)	968.97
3	Pb-214 (U-238)	295.21	11	Bi-214 (U-238)	1120.29
4	Ac-228 (Th-232)	338.32	12	K-40	1460.83
5	Pb-214 (U-238)	351.92	13	Bi-214 (U-238)	1764.40
6	Tl-208 (Th-232)	510.77	14	Bi-214 (U-238)	2204.21
7	Tl-208 (Th-232)	583.19	15	Bi-214 (U-238)	2447.86
8	Bi-214 (U-238)	609.31	16	Tl-208 (Th-232)	2614.53

¹ Errors are reported as percentage for consistency with previous work.

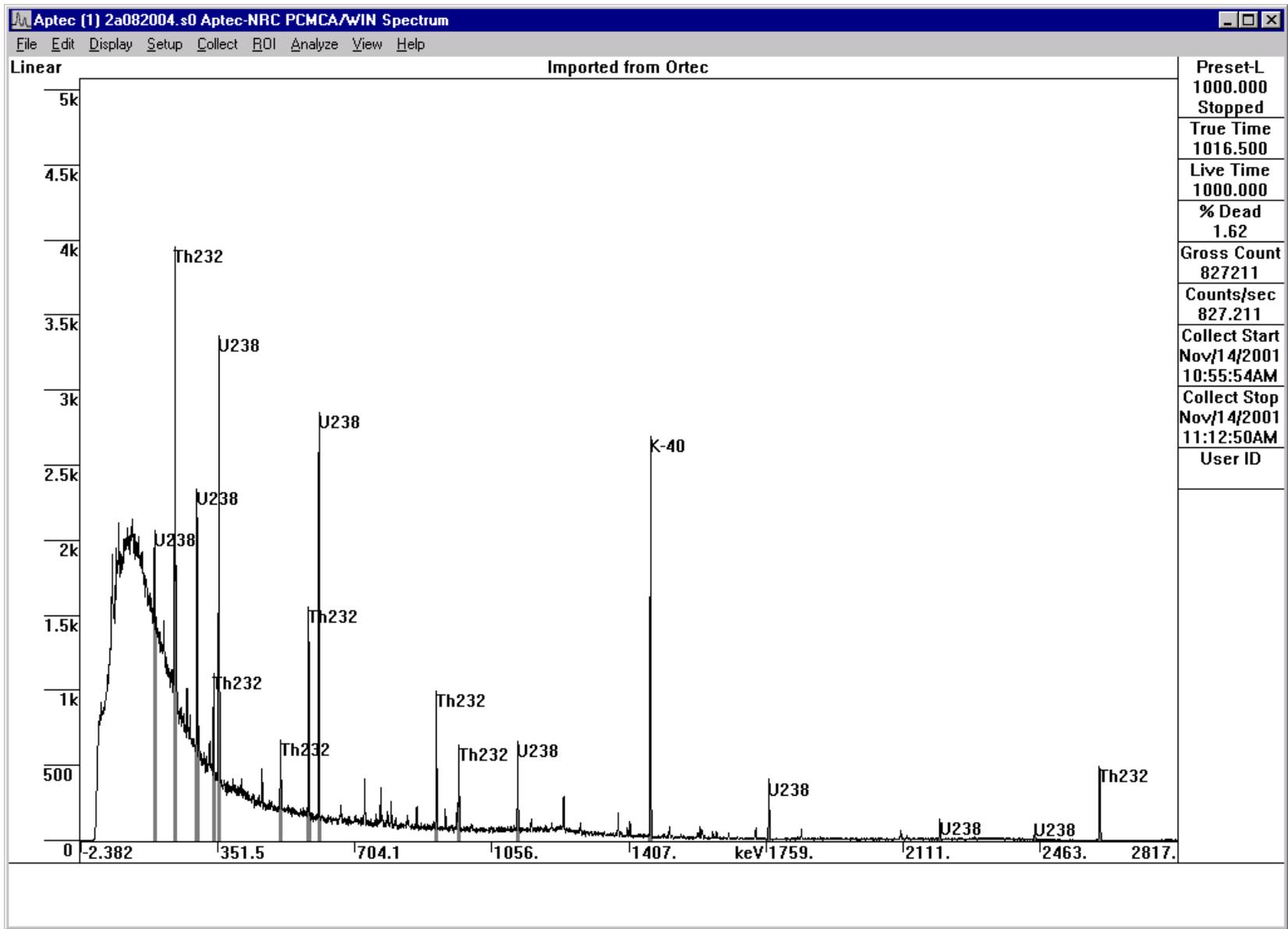


Figure 3-1. Typical SGLS Verification Spectrum

error for a region of interest (ROI) that will be accepted as a peak. For verification spectra, peaks should be reasonably well defined. An initial value of 50% is recommended. This should be adequate to detect all peaks used for energy calibration and verification tracking (see Table 3-1). If not, try increasing the value. If too many of the smaller peaks are detected, try decreasing the value.

3. Energy Calibration. Press the space bar repeatedly to index the cursor on the right-most (highest energy) ROI. This should correspond to the ^{208}Tl peak at 2614.53 keV. Use Setup/Quick Energy Calibration [F2] to enter energy values listed in Table 3-1. By starting at the highest energy, a preliminary linear calibration can be established to help identify the remaining peaks. Press the space bar to move to the left-most (lowest energy) ROI, which should be the ^{226}Ra peak at 186.10 keV. Continue advancing from left to right, entering energy values from Table 3-1 until all 16 peaks have been entered. Minor peaks not used in the calibration may be deleted using ROI/Delete Indexed [Del]. Select a 3rd order fit for the final energy calibration. Use Display/Energy Calibration to examine the calibration relationship. (Make sure the vertical scale is linear). Energy calibration details can be viewed from Setup/Full Energy Calibration. The maximum total error for the energy calibration should be less than 0.1 %.
4. Resolution Calibration and Multifit. In contrast to prior practice, a resolution calibration is not explicitly performed. When *Multifit* is run for the first time it will automatically perform a first order resolution calibration. This has been found to provide consistent and reliable results. After completing peak search and energy calibration, use Analyze/Multifit to fit a Gaussian (normal) distribution to each peak. Display/Resolution Calibration and Setup/Full Resolution Calibration can be used to evaluate the resolution calibration. Total error should be less than 4%. If necessary, a manual resolution calibration can be performed. If the resolution calibration is changed, re-run *Multifit*.
5. Peak Identification. Use Analyze/Identify Peaks to identify peaks in the verification spectrum. Note that a different library (KUT.LIB) is used for verification spectra. This is because there are several instances in which man-made and natural gamma lines are relatively close together. KUT.LIB gives preference to natural gamma lines, while SGLS.LIB gives preference to man-made gamma lines.
6. Print Peak Listing and Save Spectrum. Use File/Preview Spectrum Listing [Ctrl+Shift+F12] to display the spectrum listing. Use Setup/Listing [F2] to set the listing parameters in accordance with Table 3-1. Use File/Save Listing As to save the listing as a *.LST file and File/Print to print the listing. Finally, use File/Save As to save the spectrum in *Aptec* (*.S0) format.

3.2.2 Comparison with SGLS Verification Criteria

For the SGLS, the three most prominent peaks are chosen for verification. These are: the 609.32-keV ^{214}Bi peak, the 1460.83-keV ^{40}K peak, and the 2614.53-keV ^{208}Tl peak. Spectra are processed in accordance with Section 3.2.1. When the verification spectrum listing has been printed, highlight the peak (net) cps and FWHM values for the 609.32-keV (^{238}U), 1460.83-keV

(⁴⁰K), and 2614.53-keV (²³²Th) peaks on the printout. Compare these values to the corresponding verification criteria. Any values that fall outside the control limits should be circled in red ink.

For the SGLS, verification spectra serve two purposes. The first is to demonstrate the long-term stability of the logging system. The second is to assess the variation that may have occurred over the course of the logging day. The upper and lower control limits represent the “3-sigma” range within which nearly all data should fall. Pre-run verification spectra are compared directly to the control limits. Post-run verification spectra offer an opportunity to assess the performance of the system over the logging run. Experience has shown that FWHM values remain relatively stable, but that detector efficiency tends to decrease slightly over a typical logging day. Therefore, peak cps values for post-run verification spectra are compared to the corresponding values from the pre-run verification spectra. Net counts per second for each verification peak should be within 10% of the pre-run value. FWHM values for post-run verification spectra are compared to the appropriate control limits.

The fact that a parameter fails to meet verification criteria as described above is not necessarily an indication of system failure. Variations in system performance may be the result of variations in background radioactivity levels and/or changes in ambient conditions. When one or more verification parameters fall outside the verification criteria, the analyst should carefully examine the verification spectrum. Check the shape of the background function through the affected peak. Look for evidence of man-made radionuclides (especially ¹³⁷Cs at 661.62 keV) that may be affecting the spectra. Use the *Analyze/Compare* function to overlay other verification spectra and look for any significant differences. Check to ensure that the energy calibration is correct, that the three verification peaks are well-defined, and that there are no “tail” peaks. Check to ensure that no errors were made in processing. If there are no obvious errors and the spectrum is comparable to other verification spectra, it may be provisionally accepted. When verification peak intensity and/or FWHM fail to meet the criteria, it will be noted in the Log Data Report and a brief explanation as to the reliability of the log data will be provided. If necessary, the logging system will be checked for proper function. In some cases it may be necessary to re-log all or part of a borehole.

3.3 HRLS Verification

When the HRLS is engaged in routine operations, field verification spectra are acquired with a specially fabricated field verifier, which consists of a 200-microCurie ¹³⁷Cs source mounted in the side of a steel “pig” that surrounds the sonde in the vicinity of the detector. This was done because commercially available field verifiers designed for conventional gamma-ray logging do not provide gamma lines of sufficient intensity. Figure 3-2 illustrates a typical HRLS verification spectrum.

The HRLS field verifier presents two unique concerns. A point source is used that is located relatively close to the detector, such that minor variations in source to detector spacing may result in detectable changes in peak activity. Therefore, it is important that the logging sonde be consistently positioned in the field verifier. In addition, ¹³⁷Cs has a relatively short half-life (30.07 years) so that the peak intensity decreases over time. Over the course of a year, natural radioactive decay will result in a decrease of about 2.3% in peak activity.

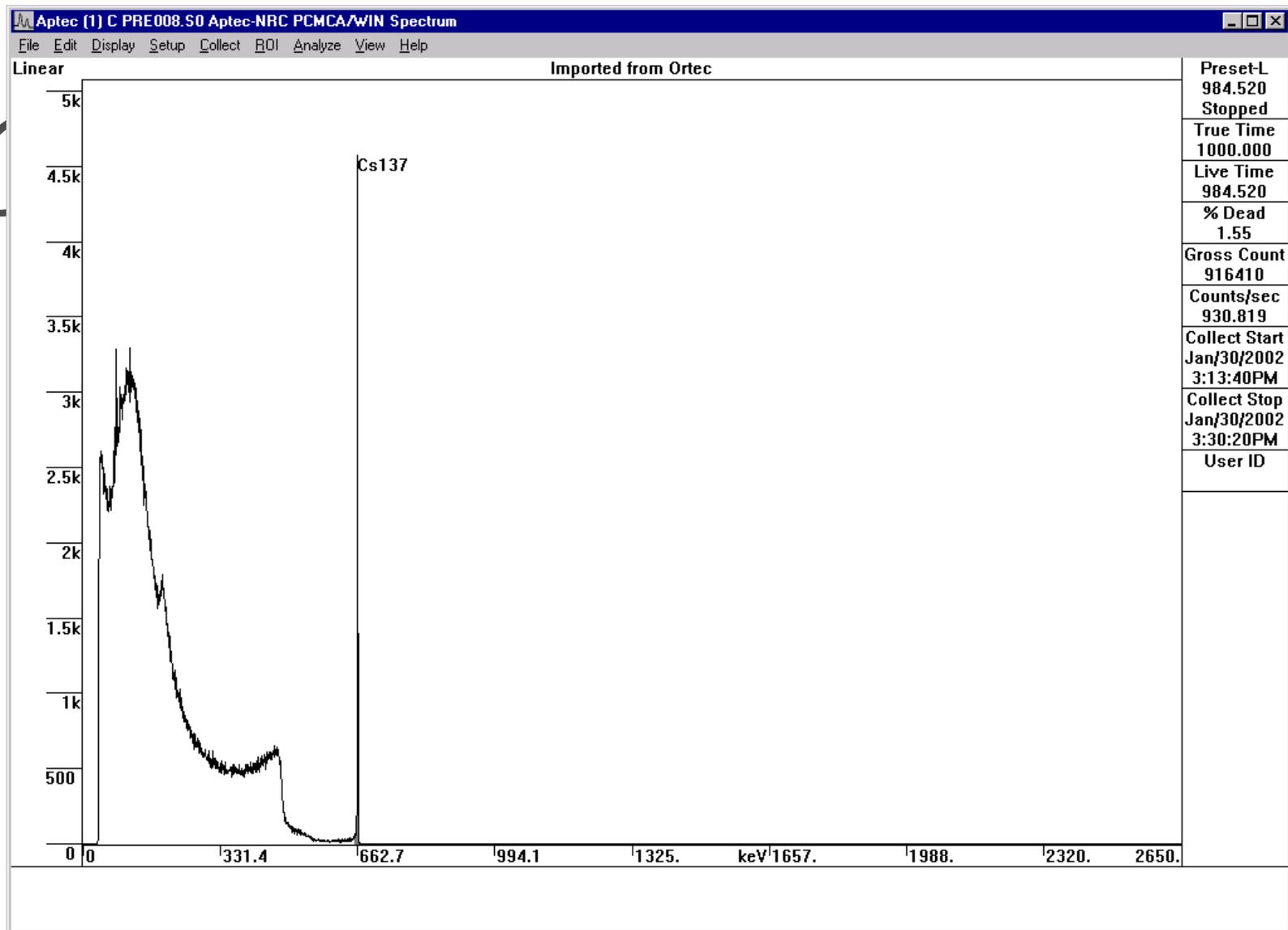


Figure 3-2. Typical HRLS Verification Spectrum

3.3.1 Processing HRLS Verification Spectra

Analysis of HRLS verification spectra generally follows the procedure outlined above for SGLS spectra, using parameters from Table 3-2. However, there are several notable exceptions. A 1st order (linear) energy calibration is used, based on the 661.62-keV peak for ¹³⁷Cs. *Multifit* is not used, and a resolution calibration is not required. Logging system performance evaluation is based on net counts (intensity) and full width at half maximum (FWHM) for the 661.62-keV peak for ¹³⁷Cs.

1. Set Up Analysis Parameters. Load the verification spectra (*.CHN) into *Aptec PCMCA/Win* software. Analysis parameters for HRLS verification spectra are provided in Table 3-2. These parameters can be entered in one of two ways as described in the SGLS discussion.
2. Perform Peak Search. Use *Analyze/Peak Search* to locate spectral peaks. Verify that Peak Search locates the ¹³⁷Cs peak.
3. Energy Calibration. Index the cursor on the ROI for the ¹³⁷Cs peak at 661.62 keV. Use *Setup/Quick Energy Calibration* [F2] to enter the energy values and select a 1st order fit for the final energy calibration.
4. Peak Identification. Use *Analyze/Identify Peaks* to identify peaks in the verification spectrum. Use the HRLS.LIB library file.
5. Print Peak Listing and Save Spectrum. Use *File/Preview Spectrum Listing* [Ctrl+Shift+F12] to display the spectrum listing. Use *Setup/Listing* [F2] to set the listing parameters in accordance with Table 3-1. Use *File/Save Listing As* to save the listing as a *.LST file and *File/Print* to print the listing. Finally, use *File/Save As* to save the spectrum in *Aptec* (*.S0) format.

3.3.2 Comparison to HRLS Verification Criteria

When the verification listing has been printed, highlight the peak (net) cps and FWHM values for the 661.62-keV ¹³⁷Cs peak and compare the values to the corresponding verification criteria. Any values that fall outside the control limits should be circled in red ink.

For the HRLS, both pre-run and post-run verification spectra are compared to the control limits. The fact that a parameter fails to meet verification criteria is not necessarily an indication of system failure. Variations in system performance may be the result of variations in background radioactivity levels and/or changes in ambient conditions. When a verification parameter falls outside the control limits, the analyst should carefully examine the verification spectrum. Check the shape of the background function through the affected peak. Use the *Analyze/Compare* function to overlay other verification spectra and look for any significant differences. Check to ensure that the energy calibration is correct and that the ¹³⁷Cs peak is reasonably well defined. Check to ensure that no errors were made in processing. If there are no obvious errors and the spectrum is comparable to other verification spectra, the spectrum may be provisionally

Table 3-2. Aptec Parameters for Processing HRLS Verification Spectra

Parameter	Recommended Value
ROI Properties	
ROI Bkgnd Line	Least-squares fit, deg 3
Use Method 2	no
Centroid Calculated	Between Net Half Max
Centroid Weighing	Net*abs(Net)*Chan
Confidence	MDA Sigma = 1.645 Error Sigma = 2
FWHM & FWTM Car	Not used
ROI Bkgnd End Points	10 End Channels (both sides)
Peak Search	
Channel Range	300-3000
Max Peak Error	10%
Smooth Before Fitting	Do not check any boxes
Energy Calibration	
Calibration Points	Cs-137 @ 661.62 keV
Max Degree	1
Multifit	
	<i>Multifit is not used for analysis of HRLS data</i>
Peak Identification	
Library	HRLS.LIB
Match ROI Centroid	Tolerance 3-4 keV
Half Life limit	Not used
Fraction Limit	5% (use a low value to "turn off" this function)
Create "Force MDA"	no
ROI Identification	Identify all ROIs
Spectrum Listing	
Include	Header, Activities with FWHM
Sort Isotopes	Alphabetically
Report Errors As	Percentage
Save Listing File	ANSI(Windows)

¹ Errors are reported as percentage for consistency with previous work.

accepted. When verification peak intensity and/or FWHM fail to meet the criteria, it will be noted in the Log Data Report and a brief explanation as to the reliability of the log data will be provided. If necessary, the logging system will be checked for proper function. In some cases it may be necessary to re-log all or a portion of a borehole.

3.4 NMLS Verification

For the neutron moisture log, verification spectra are recorded in the source shield, which yields a consistent response. No spectral processing is required. Compare the gross count rate to the verification criteria.

3.5 RAS Verification

RAS verification measurements are made in a conventional field verifier similar to that used for the SGLS. However, RAS detector response is stated in terms of total counts and gross counts

within specific energy windows, which are stated in terms of channels. Evaluation of verification spectra consists of comparing individual window count values to the average of accumulated values. Criteria are stated in terms of a 3-sigma difference from the mean. Two factors complicate this analysis. The first is that the RAS typically is located within tank farms, and many verification measurements are made in areas of high background radioactivity. This may result in anomalously high total counts and window counts. Verification spectra are first evaluated in terms of total count rate and/or dead time, and those verification spectra collected in areas of high background are not compared to the criteria. In addition, the counts in specific windows may be affected by an incorrect gain setting or gain drift. Verification spectra are evaluated to determine the centroid of a marker peak, such as the 1460.83-keV line for ^{40}K . Verification spectra that exhibit incorrect gain or excessive gain drift are eliminated from the dataset used to calculate control limits.

Failure to meet verification criteria is not by itself an indication of system failure. The logging engineer and/or analyst are responsible for evaluating suspect verification spectra in detail. Verification spectra may be provisionally accepted if it can be determined that system performance has not been seriously compromised. In some cases it may be necessary to re-log all or part of a borehole.

4.0 Log Data Processing and Analysis

Data processing and analysis refer to the conversion of raw data collected by borehole geophysical logging systems into more meaningful data that can be used for site investigation, characterization, or monitoring. The process includes data analysis using consistent methods and parameters, applying calibration functions and environmental corrections, and providing the data in a usable output format for plotting. The same software and overall approach are used for processing SGLS, HRLS, and NMLS data: specific steps, parameters, calibration, and correction functions are unique to each type of logging system. A logging system is defined as a combination of a downhole sonde with a logging unit containing a draw works, power supply, and surface electronic equipment for data collection and storage. Each sonde and logging unit is uniquely identified, and each combination represents a unique system. Table 2-1 identifies logging systems currently in use. Each system has a unique calibration function, although other functions, such as dead time correction or environmental corrections may be common to multiple systems of the same type.

A general discussion of gamma spectrum analysis is provided in Appendix B. A user guide describing various parameters controlling the analysis software is provided in Appendix C.

The following sections include specific data processing instructions for each type of logging system.

4.1 Spectral Gamma Logging System (SGLS)

4.1.1 Verification

Verification measurements are collected before and after each day's logging event to assess system performance. The verification measurements typically are analyzed in the field according to the procedures set forth in Section 3.0, "Verification Data Processing and Evaluation." Processed verification spectra are used to establish energy and resolution calibrations that are applied to each spectrum during data processing.

4.1.2 SGLS Data Processing

A typical borehole log run may contain more than 100 individual spectra, and several log runs may be required in a single borehole. The *Aptec OSQ/SUPERVISOR* program provides the capability to automate processing of gamma spectra in batch mode. This program allows the user to set up parameters for *PCMA/WIN* that determine how the region of interest (ROIs) are defined and how the subprograms *Peak Search*, *Multifit*, *Identify Peaks*, and *Spectrum Listing* functions are run. *Supervisor* applies these parameters to all selected spectra without operator intervention. With this batch processing technique, the analyst can make a first run with identical parameters applied to all spectra and then sequence through the results of each analysis to evaluate and correct

any anomalies such as unidentified peaks or false peaks. Routine processing and analysis of SGLS data consist of the following steps.

1. Set Up Files. Copy field files from the network server and set up working directories as discussed in Section 2. Review *borehole_FIELD.DOC* to determine borehole conditions and logging notes and observations. Collect any additional files that may be needed for analysis. Copy the relevant sections of *borehole_FIELD.DOC* to *borehole.DOC* and make any necessary changes or additions. Review verification spectra and verification spectra listings to determine the suitability of the verification spectra for analysis. If necessary, process any verification spectra per procedures in Section 3.
2. Batch Processing. Run *Aptec Supervisor*. Use *File/Supervisor Access* and *Edit* to set up parameters for the batch run. Recommended parameters for batch processing using *Supervisor* are provided in Table 4-1. Recommended parameters for spectral analysis are provided in Table 4-2. After analysis parameters have been set in *Supervisor*, save the *.JOB file in the working directory using *File/Save As*. Execute *Supervisor* using *Run*. In the “Open Spectrum File” dialog box select the correct directory and use the drop list under “List Files of Type” to select Ortec spectra (*.CHN). Select the appropriate spectra from a specific log run. Each log run should be analyzed independently, using either the pre-run or post-run verification spectrum associated with that run for energy and resolution calibration. In cases where gain drift has occurred, it may sometimes be necessary to process part of the run with the pre-run verification spectrum and part with the post-run spectrum. In extreme cases, it may be necessary to set up an energy calibration from one of the log spectra and use that to process part of the log run. *Supervisor* will generate *.S0 and *.LST files for each *.CHN file.
3. Review Spectral Analysis Results. After the borehole data for a log run have been processed, run *Aptec* and review individual spectra (*.S0) files. *.LST files may be reviewed using a text editor. Typical checks made during this review are discussed in Table 4-3. Make any necessary changes and use *Aptec* to modify the *.S0 file generated by *Supervisor* as necessary. If a spectrum file (.S0) is modified, the existing *.S0 file must be overwritten using the *Save* command and the corresponding *.LST file must also be overwritten by using *File/Preview Spectrum Listing* [Ctrl+Shift+F12], followed by *File/Save As*. When all spectra have been reviewed, the analyst can also run *LISTEM.BAT* to generate *.LST files from the most recent *.S0 files.

Table 4-1. Aptec *Supervisor* Parameters for Processing SGLS Spectra

Parameter	Recommended Value
Title	Based on borehole number
Data Source	Spectrum File (only available option)
Reset Header	Not used
Embed Header into Job	
Embedded Calculations	
Efficiency	Not used
Energy	
Resolution	
Job Environment	
Recycle	Not available
ROI Properties	✓ Use >>Setup to set parameters per Table 4-2
Sample	Not used
Quantity	
Password	
Run Sequence	
Instructions	Not used
Setup App	
Link at Run Time	
Use Sample/Quantity Info	Select "from this job"
Use Efficiency Calibration	
Use Energy Calibration	Select "or from file" and designate the appropriate verification
Use Resolution Calibration	spectrum
Use ROIs	Select "from this job"
Do Collection	Not available
View While Collecting	
Search	✓ Use >>Setup to set parameters per Table 4-2
Multifit	✓ Use >>Setup to set parameters per Table 4-2
Identify	✓ Use >>Setup to set parameters per Table 4-2
Bkgnd Subtract	Not used
Quantify	
Print Listing	Do not check, but use >>Setup to set parameters per Table 4-2
Print Report	Not used
Save	
Spectrum Name	Aptec always uses the name of the spectrum file
Save Spectrum	✓ Select Aptec spectra (* 80)
Save Listing	✓ (Set parameters per Table 4-2 under >>Setup for Print Listing)
Save CSV Listing	Not used
Save Process Report	
Append QA/QC Info	
Final App	Not used
When Done	
Select either "Exit" or "Wait", depending on requirements. "Exit" terminates the program and "Wait" allows the analyst to change parameters and make another run.	

Table 4-2. Aptec Parameters for Processing SGLS Spectra

Parameter	Recommended Value
ROI Properties	
ROI Bkgnd Line	Least-squares fit, deg 2
Use Method 2	X (yes)
Centroid Calculated	Between Net Half Max
Centroid Weighing	Net*abs(Net)*Chan
Confidence	MDA Sigma = 1.645 Error Sigma = 2
FWHM & FWTM Cal	Use least-squares fit
ROI Bkgnd End Points	10 End Channels (both sides)
Peak Search	
Channel Range	150-4095
Max Peak Error	50%
Smooth Before Fitting	Do not check any boxes
Energy Calibration	
<i>Imported from verification spectrum under "Link at Run Time"</i>	
For individual spectra, use <u>Edit/Load Header Information</u> , designate the appropriate spectrum, and select "Energy Calibration"	
Resolution Calibration	
<i>Imported from verification spectrum under "Link at Run Time"</i>	
For individual spectra, use <u>Edit/Load Header Information</u> , designate the appropriate spectrum, and select "Resolution Calibration"	
Multifit	
Spectrum Type	HPGe/GeLi
Optimize Centroid Search for	Separated Overlaps ¹
Peaks to be Fitted	Multiplets & Singlets Sigma = 1.645
Fit Parameters	Fit with Peak Width: Fixed Fit with Background: Fixed
Accuracy	Maximum Iterations = 20-40 Maximum Overlaps = 4-5 Percent Change = 0.25 Minimum Reduced Chi Square = 0.75
Peak Identification	
Library	SGLS.LIB
Match ROI Centroid	Tolerance 3-4 keV
Half Life limit	Not used
Fraction Limit	5%
Create "Force MDA"	Yes (for Cs-137, KUT) with ROI width of 2.55 times its FWHM ³
ROI Identification	Identify all ROIs
Spectrum Listing	
Include	Header, Activities with MDA, Activities with FWHM
Sort Isotopes	Alphabetically
Report Errors As	Percentage ²
Save Listing File	ANSI (Windows)

¹ "Close Overlaps" may be selected when peaks are skewed by pulse pileup.

² Errors are reported as percentage for consistency with previous work.

³ The default value of 2.07892 is what previous versions of S_Ident used and is equivalent to full width 20th max. It is suggested that a value of 2.55 times the FWHM is more appropriate as this gives 95% of the area of a Gaussian peak.

Table 4-3. Guidelines for SGLS Spectral Analysis

Checks	Discussion
Assure 609-, 1460-, 1764-, 2615-keV peaks are identified	Typical counting errors (100-s count time in 6-in. casing) are about 15, 30, 40, 40 percent, respectively. Error can vary considerably depending on counting time and casing thickness.
Misidentified Peaks	System gain drift causes energy calibration to be out of 3- to 4-keV tolerance. Requires new energy calibration for affected spectra.
Interferences	Most common interfering peaks occur near 510 keV (^{228}Ac , ^{106}Ru , and annihilation peak), 1001-1004 keV (^{234}Pa , ^{154}Eu), 186 keV (^{226}Ra and ^{235}U), 1460 keV (^{228}Ac , ^{40}K). Secondary peaks should be looked for if the analyst is in doubt.
Spurious Peaks	Often occur on the downside tails of larger peaks and can be erroneously identified as the large or "parent" peak. The small peak is deleted and peak identification rerun.
High Concentrations of Radionuclides	In zones of high ^{137}Cs concentrations the spectra become distorted by pulse pileup and an elevated Compton continuum that may cause multiple peaks to be identified. Peaks identified in this instance typically can be deleted. No special manual efforts such as painting ROIs to consolidate multiple peaks in the 662-keV energy range are required. High rate logging is recommended where dead time exceeds 40 %.
Confirmation Peaks	Peaks of man-made radionuclides identified near their MDL by routine processing require verification. Check that confirming peaks are present in spectrum (e.g., 1004 and 1275 keV for ^{154}Eu). In addition, it should be expected that a legitimate peak would be detected at two or more consecutive depths. Delete a peak if it cannot be confirmed.
Associations	It is common for some radionuclides to be associated such as ^{234}Pa usually exists with ^{235}U and ^{152}Eu with ^{154}Eu . Consider confirmation peaks also if the legitimacy of a peak is in question.
Radon	Radon in the borehole can affect ^{238}U concentrations. Analyst should consider the existence of the 295-keV energy peak at normal counting times as an indicator of ^{222}Rn . A systematic difference in total gamma count rate in repeat sections is also an indicator.
KUT Concentrations	If the KUT concentrations deviate significantly from normal background concentrations, the analyst should note that casing configuration or grout around the borehole may be affecting the log data.

4. Generate Log Data Files. The *.S0 and *.LST files contain the results of spectral analysis for individual log spectra. It is necessary to collect the data from these files and write it to data files as a function of depth, which is embedded in the Sample ID field. *SGLSoffline* is an in-house program that reads individual spectrum files and writes a series of *.RAS files in text format. Most of these files have a name of the form *eeee.RAS*, where *eeee* indicates the energy level of a specific gamma peak. For example 1173.RAS contains data for the ⁶⁰Co peak at 1173.24 keV (there should also be a 1332.RAS file if ⁶⁰Co is present). Data fields in the *.RAS file are fixed length. Columns in an *eeee.RAS* file are:

- depth measurement depth (ft)
- deadtime percent dead time
- cps net count rate for peak
- cpsUnc uncertainty in net count rate (in percent)
- mda minimum detectable activity
- flag flag indicating type of value
- filename spectrum file name

The file GROSSCNTS.RAS contains total count data organized in columns as follows:

- depth measurement depth (ft)
- cps net count rate for peak
- true time true time (sec)
- live time live time (sec)
- deadtime percent dead time
- gross cnts total gross counts

4.1.3 Calculate Concentrations

Radionuclide concentrations, concentration error, and minimum detectable level (MDL) are reported in units of picocuries per gram (pCi/g). These quantities are determined from peak data by:

$$C_a = \frac{27.027}{Y} \times I(E) \times K_w \times K_c \times DTC \times n$$

$$u(C_a) = \frac{27.027}{Y} \times I(E) \times K_w \times K_c \times DTC \times u(n)$$

$$MDL = \frac{27.027}{Y} \times I(E) \times K_w \times K_c \times DTC \times MDA$$

Where *n* is the net count rate, *u(n)* is the uncertainty in count rate, and *MDA* is the minimum detectable activity for the specific peak. All these values are in units of counts per second (cps). *I(E)* is the detector calibration function (inverse efficiency as a function

of energy level, expressed in gammas per second per gram per count per second), Y is the radionuclide yield (gammas per decay), DTC is the dead time correction, and K_c and K_w are casing and water corrections, respectively. The factor 27.027 is the conversion between decays per second and picocuries (10^{-12} Curies). Tables 4-4 and 4-5 provide peak energy and yield values for commonly encountered natural and man-made radionuclides.

Concentrations calculated from SGLS data are made on the assumption of a uniformly distributed homogeneous distribution around the borehole axis, and that the sonde axis is coincident with the borehole axis. Because these conditions are not necessarily true, the concentrations calculated from log data should be considered "apparent" concentrations. In addition, the error calculated above reflects only the error resulting from the statistical nature of radioactivity, and does not take into account errors in the calibration function, errors in environmental correction functions, or variability associated with nonconformity to the assumed contaminant distribution.

Given below is a brief discussion of the functions involved in the concentration calculation.

- **Calibration Function.** $I(E)$ describes the response of the SGLS detector as a function of energy level. Each detector-logging unit combination (system) has a unique calibration function, which is updated annually. The calibration function is described in Appendix B. The constants for a specific system are reported in the corresponding calibration certificate.
- **Dead Time Correction.** The dead time correction accounts for the fact that the system cannot process all charge pulses when high gamma flux is encountered. The dead time is expressed as a percentage, and may range from zero to 100%. At 100% dead time, the detector is "saturated" and no counts are recorded. The dead time correction function is described in Appendix B. Each logging unit has a unique dead time correction function. A dead time correction is applied when the dead time exceeds 10.5%. For the SGLS, the dead-time correction is considered acceptable up to about 70%, but peak spreading, pulse pileup and pulse rejection contribute to severely distorted peaks, and concentration is likely to be underestimated for dead times greater than about 40%. The HRLS is recommended for logging when SGLS dead times exceed 40%.
- **Casing Correction.** A casing correction is required to account for the fact that gamma radiation is attenuated as it passes through steel casing. The degree of attenuation is dependent on both gamma energy level and casing thickness. A generalized casing correction has been developed for all SGLSs. This is described in Appendix B. For gamma energies greater than 600 keV, the casing correction function can be used for casing thickness as much as 2 in.

Table 4-4. Naturally Occurring Radionuclide Data

Radionuclide	Primary Gamma Rays			Secondary Gamma Rays		
	Daughter	E (keV)	Y (%)	Daughter	E (keV)	Y (%)
⁴⁰ K		1460.83	10.67			
²³² Th	²⁰⁸ Tl	2614.53	35.34	²¹² Pb	238.63	43.30
				²⁰⁸ Tl	583.19	30.11
				²²⁸ Ac	911.21	26.60
				²²⁸ Ac	968.97	16.17
				²²⁸ Ac	338.32	11.25
				²⁰⁸ Tl	510.77	8.06
²³⁸ U ¹	²¹⁴ Pb ²¹⁴ Bi	609.31	44.79	²¹⁴ Pb	351.92	35.80
		1764.49	15.36	²¹⁴ Pb	295.21	18.50
				²¹⁴ Bi	1120.29	14.80
				²¹⁴ Pb	241.98	7.50
				²¹⁴ Bi	1238.11	5.86
				²¹⁴ Bi	2204.21	4.86
				²¹⁴ Bi	2447.86	1.50

¹ Attainment of secular equilibrium between ²³⁸U and ²¹⁴Bi/²¹⁴Pb requires time periods on the order of several million years. Activities of both ²¹⁴Bi and ²¹⁴Pb are commonly assumed to be equal to the activity of naturally occurring ²³⁸U. However, these radionuclides are short-term daughter products of ²²²Rn, and accumulations of radon gas inside the casing may temporarily perturb the secular equilibrium between ²³⁸U and ²¹⁴Bi/²¹⁴Pb.

Table 4-5. Man-Made Radionuclide Data

Radionuclide	Half Life (Years)	Primary Gamma Rays		Secondary Gamma Rays	
		E (keV)	Y (%)	E (keV)	Y (%)
^{60}Co	5.2714	1332.50 1173.24	99.98 99.90		
^{106}Ru	1.0238	511.86	20.40	621.93	9.93
^{125}Sb	2.7582	427.88	29.60	600.60 635.95 463.37	17.86 11.31 10.49
^{126}Sn	1.E+05	414.50	86.00	666.10 694.80	86.00 82.56
^{134}Cs	2.062	604.70	97.56	795.85	85.44
^{137}Cs	30.07	661.66	85.10		
^{152}Eu	13.542	1408.01	20.87	121.78 344.28 964.13 1112.12 778.90	28.42 26.58 14.34 13.54 12.96
^{154}Eu	8.593	1274.44	35.19	123.07 723.31 1004.73 873.19	40.79 20.22 18.01 12.27
^{155}Eu	4.7611	105.31	21.15		
^{235}U	7.04E+08	185.72	57.20		
$^{234\text{m}}\text{Pa}$ (^{238}U) ¹	4.47E+09	1001.03	0.84	811.00 766.36	0.51 0.29
^{237}Np	2.14E+06	312.17	38.60		
^{239}Pu	24110	129.30 375.05 413.71	0.0063 0.0016 0.0015		
^{241}Am	432.2	59.54	35.90		

¹ $^{234\text{m}}\text{Pa}$ is a short-term daughter of ^{238}U . Secular equilibrium is achieved relatively quickly. Because of the relatively low gamma yield, this peak is not observed when only background levels of naturally occurring ^{238}U are present. Hence, the presence of gamma peaks associated with $^{234\text{m}}\text{Pa}$ without corresponding peaks associated with ^{214}Pb and ^{214}Bi is taken as an indication of man-made or chemically processed uranium.

- Water Correction. A water correction is required to account for the additional gamma attenuation associated with water in the annulus between the sonde and the borehole wall. A generalized water correction has been developed for all SGLS systems as described in Appendix B. Note that the water correction function does not account for the effects of water in the pore space. Hence, concentrations below the groundwater level will be slightly underestimated.
- Shield Correction. A tungsten sleeve, known as the external shield, can be installed on the outside of the sonde to reduce count rates. The shield correction, described in Appendix B, is a function of shield thickness and gamma energy level. The shield is seldom used with the SGLS; when high dead times are encountered, the HRLS is recommended for logging.

The above calculations are carried out in an *Excel* workbook. Preliminary plots can also be generated from *Excel*. The process for calculating concentrations follows these steps:

1. Setup *Excel* Workbook. In *Excel*, open the correct template workbook for the logging system in use. Immediately save the workbook under the borehole directory to avoid corrupting the template. The workbook includes worksheets for *I(E)*, dead time correction, casing correction, and water correction, as well as individual worksheets for each radionuclide. The radionuclide worksheets are identified by *eee*, where *eee* indicates the peak energy. Each *.RAS file imported into *Excel* should have a corresponding worksheet in the log analysis workbook. Within the workbook, links and lookup functions are used to avoid duplicate data entry. Worksheet protection is invoked to prevent inadvertent alteration. A *Description* page contains a detailed description of the worksheet and specific instructions. Borehole details, such as borehole name, casing thickness and depth, borehole diameter, and depth to water are entered on the *Summary* worksheet. All depths are entered relative to the depth reference, which generally will be top of casing (TOC) in existing boreholes. Ground surface may be used for temporary boreholes, or where permanent casing has not yet been installed. Note that the thickness values entered on the summary page are not individual casing thickness, but cumulative thickness. For example, consider the case where 8-in.-diameter, 0.322-in.-thick casing extends from the ground surface to 50-ft depth and 6-in.-diameter, 0.280-in.-thick casing extends from the ground surface to 100-ft depth. The values entered on the *Summary* worksheet would be 0.602 (0.322+0.280) in. for 0 to 50 ft and 0.280 in. for 50 to 100 ft. Data for selected radionuclides are entered on the *I(E)* worksheet. Each radionuclide worksheet contains a specific energy value in cell I1, which is used to look up energy-dependent values for concentration calculations. The energy value entered here must correspond to one of the energy values in cells B11 to B30 on the *I(E)* worksheet.

Note: Occasionally, when boreholes are logged during drilling, there may be several logging events, each with a different casing configuration. When this

occurs the analyst should develop a separate workbook for each logging event, and combine the data for plotting.

2. Load Data and Calculate Concentrations. To import data from *eee.RAS*, use the *File/Open* command in *Excel* and select the correct *.RAS file. This will invoke the File Import Wizard, which will load the data into a new *Excel* file. Copy columns A through G onto the corresponding *eee* worksheet in the analysis workbook. Each *eee* page is organized so that columns A through G contain input data, column H is blank as a “buffer,” and calculations are performed in columns I through R. Copy row 6 in columns I through R downward to the end of the data. Repeat this process for each radionuclide. *GROSSCNTS.RAS* is imported to the *grosscnts* worksheet using a similar process. Each analysis template workbook contains a series of worksheets for the most common radionuclides. These can be reconfigured and additional sheets can be added as necessary. When calculations are complete, unused radionuclide (*eee*) worksheets should be deleted.
3. Organize Data for Plotting. After all calculations are complete, copy columns O, P, Q, and R from each radionuclide worksheet to the correct columns on the *logdata* worksheet. Use the *Edit/Paste Special* command and select “values” to copy the data. Save the completed workbook as *borehole.XLS*. The *logdata* worksheet contains data that can be copied into *SigmaPlot* for plotting. Finally, add analysis notes, log plot notes, and results and interpretations to the *borehole.DOC* file, and save it in the working directory.

4.2 High Rate Logging System (HRLS)

4.2.1 Verification

Verification measurements are collected before and after each day’s logging event to assess system performance. The verification measurements typically are analyzed in the field according to the procedures set forth in Section 3.0. Processed verification spectra are used to establish energy calibrations that are applied to each spectrum during data processing. A resolution calibration is not necessary because the “multifit” routine is not used to analyze high rate data.

4.2.2 HRLS Data Processing

Aptec *Supervisor* is also used to analyze HRLS data. Tables 4-6 and 4-7 provide recommended HRLS batch and analysis parameters. The most significant differences between the SGLS and HRLS processing parameters are that the HRLS energy calibration is limited to a first-order (linear) function based on the 661.66-keV ¹³⁷Cs peak, the resolution calibration is not performed, and the Aptec *Multifit* routine is not used to fit a Gaussian distribution to the peaks because of the tailing characteristics. HRLS data generally are analyzed in conjunction with SGLS data, so that the procedure outlined under Section 4.1 is followed.

Table 4-6. Aptec Supervisor Parameters for Processing HRLS Spectra

Parameter	Recommended Value
Title	Based on borehole number
Data Source	Spectrum File (only available option)
Reset Header	Not used
Embed Header into Job	
Embedded Calculations	
Efficiency	Not used
Energy	
Resolution	
Job Environment	
Recycle	Not available
ROI Properties	✓ Use >>Setup to set parameters per Table 4-7
Sample	Not used
Quantity	
Password	
Run Sequence	
Instructions	Not used
Setup App	
Link at Run Time	
Use Sample/Quantity Info	Select "from this job"
Use Efficiency Calibration	
Use Energy Calibration	Select "or from file" and designate the appropriate verification spectrum
Use Resolution Calibration	Select "from this job"
Use ROIs	
Do Collection	Not available
View While Collecting	
Search	✓ Use >>Setup to set parameters per Table 4-7
Multifit	Not used
Identify	✓ Use >>Setup to set parameters per Table 4-7
Bkgnd Subtract	Not used
Quantify	
Print Listing	Do not check, but use >>Setup to set parameters per Table 4-7
Print Report	Not used
Save	
Spectrum Name	Aptec always uses the name of the spectrum file
Save Spectrum	✓ Select Aptec Spectra (*.S0)
Save Listing	✓ (Set parameters per Table 4-7 under >>Setup for Print Listing)
Save CSV Listing	Not used
Save Process Report	
Append QA/QC Info	
Final App	Not used
When Done	
Select either "Exit" or "Wait", depending on requirements. "Exit" terminates the program and "Wait" allows the analyst to change parameters and make another run.	

Table 4-7. Aptec Parameters for Processing HRLS Spectra

Parameter	Recommended Value
ROI Properties	
ROI Bkgnd Line	Least-squares fit, deg 3
Use Method 2	X (yes)
Centroid Calculated	Between Net Half Max
Centroid Weighing	Net*abs(Net)*Chan
Confidence	MDA Sigma = 1.645 Error Sigma = 2
FWHM & FWTM Cal	Not used
ROI Bkgnd End Points	10 End Channels (both sides)
Peak Search	
Channel Range	200-3000
Max Peak Error	80%
Smooth Before Fitting	Do not check any boxes
Energy Calibration	
<i>Imported from verification spectrum under "Link at Run Time"</i>	
Multifit	
<i>Multifit is not used for analysis of HRLS data</i>	
Peak Identification	
Library	HRLS.LIB
Match ROI Centroid	Tolerance 3-4 keV
Half Life limit	Not used
Fraction Limit	5%
Create "Force MDA"	Yes (for Cs-137)
ROI Identification	Identify all ROIs
Spectrum Listing	
Include	Header, Activities with MDA, Activities with FWHM
Sort Isotopes	Alphabetically
Report Errors As	Percentage
Save Listing File	ANSI (Windows)

¹ Errors are reported as percentage for consistency with previous work.

After the HRLS data for a log run have been processed, run *Aptec* and review individual spectra (*.s0) files. *.LST files may be reviewed using a text editor. Typical checks made during this review are discussed in Table 4-8.

The HRLS spectra and *.LST files are processed through *SGLSOffline* as described in Section 4.1.2. HRLS data files should be located in a separate subdirectory to avoid overwriting SGLS data files. After *SGLSOffline* is run to generate *eeee.RAS* files, these files should be renamed to *eeeeHR.RAS* to identify them as HRLS data.

4.2.3 Calculation of Radionuclide Concentrations

Concentrations are calculated from HRLS data using the same equations as those for the SGLS. However, there are a number of important differences:

- Cs-137. Experience has shown that ¹³⁷Cs tends to be the dominant radionuclide detected in borehole intervals with high gamma flux. Other radionuclides are

unlikely to be detected in high rate zones unless they are present at activities comparable to the ^{137}Cs concentration.

- Dead Time Correction. The HRLS dead time correction function becomes mathematically unstable at dead times greater than 70%. Dead time corrections are applied for dead times between 10.5 and 56%. Data where the dead time exceeds 56% should not be used. When dead time exceeds 30%, shields should be used.
- Casing Correction. The HRLS was calibrated with a 0.28-in. steel sleeve in place over the detector. Hence, HRLS response is normalized for a typical 6-in. schedule-40 casing. For a different casing thickness, a correction factor is calculated based on attenuation relative to 0.28 in. of steel. The HRLS casing correction factor is calculated as follows:

$$K_c = \exp(2.54\mu\rho(T - 0.280)) = \exp(1.443(T - 0.28))$$

where: μ = mass attenuation coefficient, cm^2/g (= 0.0738 at 662 keV)
 ρ = bulk density, g/cm^3 (= 7.7 for steel)
 T = casing thickness, in (1 in. = 2.54 cm)

- Water Correction. No water correction function is available for the HRLS.
- Shield Correction. Two shields are available for use with the HRLS. The first is a 0.31-in. tungsten sleeve that can be installed on the outside of the sonde. This is known as the external shield. The second is a tungsten “cup” with a wall thickness of 0.7 in. that fits over the detector inside the sonde housing. This is known as the internal shield. An energy-dependent correction function has been developed for the external shield and is described in Appendix B. No such function is available for the internal shield, but a shield correction factor has been estimated for ^{137}Cs (661.62 keV) from comparison of overlapping log runs in a borehole known to intersect high concentrations of ^{137}Cs . The empirical shield correction factors are:

- External Shield: 3.758
- Internal Shield: 27.42
- Both Shields: 96.4

Each SGLS workbook includes a worksheet for analysis of HRLS data. A separate *Excel* workbook has been developed for independent analysis of HRLS data.

Table 4-8. Guidelines for HRLS Spectral Analysis

Checks	Discussion
Assure 662-keV peak is identified	Usually only the ^{137}Cs peak is identified if low dead time.
Verify energy calibration	System gain drift causes energy calibration to be out of 3-keV tolerance. Requires new energy calibration for affected spectra.
Misidentified peaks	Seemingly legitimate peaks typically are single or double sum peaks. Library should be checked to determine validity. Delete if appropriate.
High concentrations of radionuclides	In zones of high concentrations of ^{137}Cs the spectra become distorted by pulse pileup and an elevated Compton continuum that cause multiple low energy peaks to be identified. These peaks generally can be deleted. Adding a shield is recommended where dead time exceeds 30 %.
Confirmation peaks	Unlikely in a typical spectrum except for ^{60}Co (1173- and 1333-keV peaks).

4.3 Neutron Moisture Logging System (NMLS)

The neutron moisture log primarily responds to moisture present in the surrounding formation. In general, an increase in total neutron counts reflects an increase in moisture content. Calibration functions are available for 6-in. and 8-in. boreholes. However, the NMLS is strongly affected by borehole diameter, so the analyst should not attempt to calculate moisture content when borehole diameter is significantly different from 6 in. or 8 in.

4.3.1 Verification

Verification measurements are collected before and after each day's logging event to evaluate system operating performance.

4.3.2 NMLS Data Processing

Aptec *Supervisor* is used to generate read *.CHN files generated by the NMLS and generate a *.CSV file containing Sample ID, True Time, Live Time and Gross Counts. This file can be opened by *Excel*, where depth can be extracted from the sample ID and gross count rate can be calculated. When appropriate, the calibration function can be applied to calculate moisture content. Table 4-9 lists recommended *Supervisor* parameters for NMLS data analysis.

4.4 Radionuclide Assessment System (RAS)

4.4.1 Verification

Verification measurements are collected before and after each day's logging event to assess system performance. Evaluation of verification measurements for the RAS is

complicated by the fact that many of the areas in which the RAS operates have higher than normal levels of ambient radioactivity.

4.4.2 RAS Data Processing

Processing of data with Aptec *Supervisor* is not necessary because the logging system data output is in comma-separated-value (*.csv) text files that can be readily imported into *Excel* workbooks. Although spectra are collected and stored, they are not normally analyzed.

4.4.3 Analysis - Comparison of Data from Separate Logging Events

The RAS was designed as a relatively simple logging system to detect changes in pre-existing areas of contamination. Because contaminant identification and concentration are known from the baseline data, it is not necessary that the RAS be able to identify and quantify contaminants. The RAS collects and stores 256 channel spectra in *.CHN format; these are generally not analyzed. During logging operations, the RAS software accumulates counts in eight contiguous energy windows. Window ranges were selected to detect natural radionuclides and to maximize sensitivity to man-made radionuclides. Table 4-10 shows the RAS windows in terms of both energy and channel number.

An *Excel* workbook is maintained for each borehole subject to RAS monitoring. Window counts and gross counts from successive log runs are imported into the workbook. Decay corrections are made as needed and the data from each log run are plotted as a function of depth. Evaluation of RAS data is performed primarily by visual comparison of window count rates or total count rate as a function of time. Contaminant migration is indicated by an anomalous increase in activity at several contiguous points, an increase in the extent of a contaminant interval, or downward movement of the contaminated interval. When contaminant levels at a point are observed to increase between log runs, it is necessary to determine if the increase is significant, or simply a manifestation of the normal statistical error associated with radioactive decay. Appendix E provides a discussion of the statistical basis for determining when a significant difference in count rates exists.

Table 4-9. Aptec Supervisor Parameters for Processing NMLS Spectra

Parameter	Recommended Value	
Title	Based on borehole number	
Data Source	Spectrum File (only available option)	
Reset Header	Not used	
Embed Header into Job		
Embedded Calculations		
Efficiency	Not used	
Energy		
Resolution		
Job Environment		
Recycle	Not available	
ROI Properties	Not used	
Sample		
Quantity		
Password		
Run Sequence		
Instructions	Not used	
Setup App		
Link at Run Time	Not used (Select "From This Job")	
Use Sample/Quantity Info		
Use Efficiency Calibration		
Use Energy Calibration		
Use Resolution Calibration		
Use ROIs	Not available	
Do Collection		
View While Collecting	Not used	
Search		
Multifit		
Identify		
Bkgnd Subtract		
Quantify		
Print Listing		
Print Report		
Save		Aptec always uses the name of the spectrum file
Spectrum Name		
Save Spectrum		
Save Listing		
Save CSV Listing		
Save Process Report		
Append QA/QC Info	✓ Execute Setup. Under "Include," select "Sample ID," "True Time," "Live Time" and "Gross counts." Do not select any boxes under "Include for each ROI."	
Final App	Not used	
When Done		
Select either "Exit" or "Wait", depending on requirements. "Exit" terminates the program and "Wait" allows the analyst to change parameters and make another run.		

Table 4-10. RAS Energy Windows

Window	Energy Range, keV	#	RAS Detector Channel Numbers		
			Large (L)	Medium (M)	Small (S)
lithology	0 – 570	1	0 – 50	0 – 51	0 – 51
Cs-137	570 – 740	2	51 – 64	52 – 66	52 – 66
Midrange	740 – 940	3	65 – 82	67 – 83	67 – 83
Pa-234	940 – 1060	4	83 – 92	84 – 93	84 – 93
Co-60	1060 – 1390	5	93 – 121	94 – 121	94 – 121
K-40	1390 – 1600	6	122 – 139	122 – 138	122 – 138
U-238	1600 – 2400	7	140 – 209	139 – 202	139 – 202
Th-232	2400 – 2800	8	210 – 255	203 – 255	203 – 255

5.0 Shape Factor Analysis

This section will be prepared and implemented at a later date.

6.0 Log Plotting and Reporting

This section outlines the specifications for the plotting, reporting, and file archiving of the results of the borehole geophysical logging. Examples of log plots and Log Data Reports are shown as an example of format.

6.1 Log Plotting

SigmaPlot 8.0, a program from SPSS, provides capabilities for plotting analysis results from the geophysical logging. It should be noted that any scientific graphing program can be used for this step, but the project currently uses *SigmaPlot 8.0* for consistency and continuity with data presentation in Hanford Tank Farms Vadose Zone Characterization Project documents.

SigmaPlot is used to generate log plots of radionuclide concentrations, percent dead time, percent moisture, and neutron counts or gamma-ray counts versus borehole depth. For details about the operation of *SigmaPlot*, users should consult the program's user's manual or help files.

After radionuclide concentrations or other quantities are derived from corrected log data, the quantities are imported to *SigmaPlot* from the *log data* worksheet within the *Excel* spreadsheet for the borehole. Data are imported into a spreadsheet work area within *SigmaPlot*. *SigmaPlot* is organized in a workbook fashion, with one or more sections each containing a data worksheet and one or more graph pages. Each graph page may contain several graphs, with multiple plots on each graph. A standard suite of plots has been pre-defined based upon commonly encountered radionuclides. These plots will be generated for any data imported into the *SigmaPlot* notebook template. The template ensures consistency in presentation of results from borehole to borehole. Additional plots may be necessary to fully describe borehole conditions and their selection is at the discretion of the analyst.

Examples of the various plots are provided as a guide to proper format and presentation. Figure 6-1 shows a typical gross gamma and dead time plot. Figure 6-2 shows a typical natural (KUT) plot. Figure 6-3 shows a typical man-made radionuclide concentration plot. Figure 6-4 shows a typical combination plot, and Figure 6-5 shows a typical repeat log plot.

In general, the combination plot should be plotted at a consistent scale (20 ft/in.) to facilitate comparison and correlation between boreholes. When this scale is inadequate, the analyst is free to modify scales on additional plots. Where more than one page is required, there should be an overlap of at least 10 ft in the depth range between successive log pages.

The order of the tracks on the combination plot should be consistent. There are a total of six graphs or tracks available. The first track should show man-made contaminant data. The second, third, and fourth tracks are reserved for natural radionuclide (KUT) data, and the fifth track should show total gamma data. The content of the sixth track may vary depending upon data availability. Examples of data that can be plotted in the sixth track are neutron, dead time, historical logs, and sample results.

299-E33-58 (A6866) Total Gamma & Dead Time

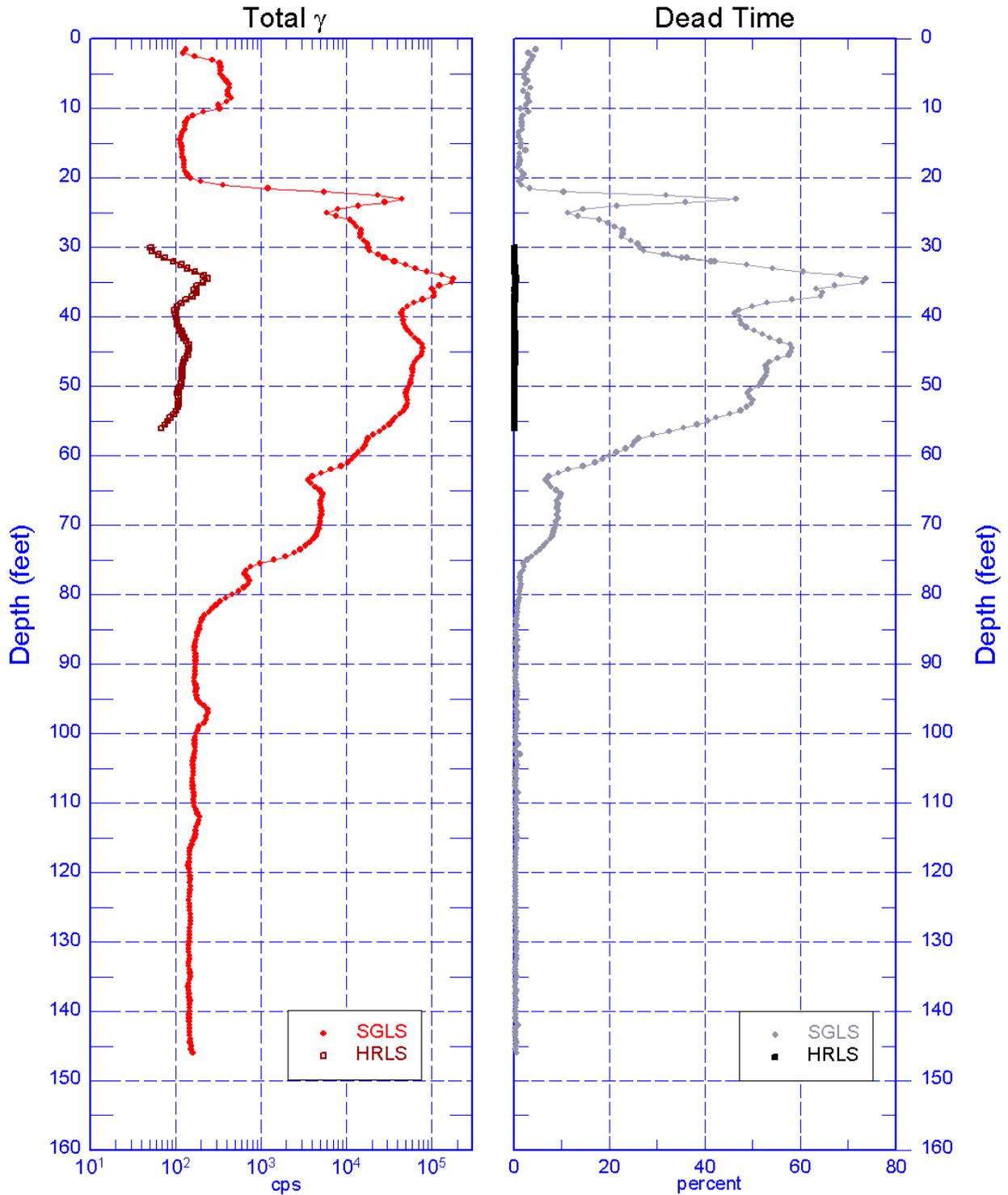


Figure 6-1. A Typical Gross Gamma and Dead Time Plot

299-E33-58 (A6866) Natural Gamma Logs

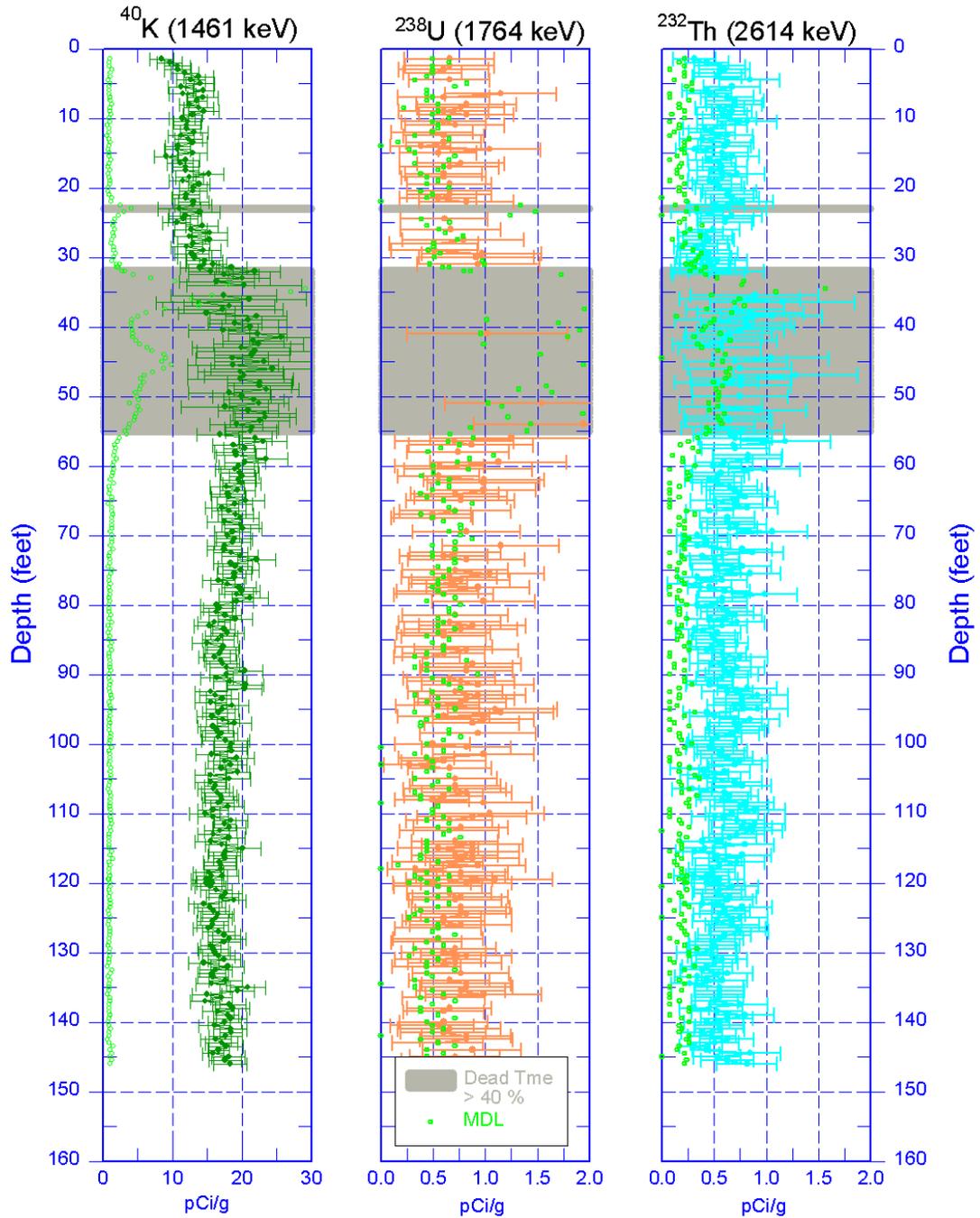


Figure 6-2. A Typical Natural (KUT) Plot

299-E33-58 (A6866) Man-Made Radionuclide Concentrations

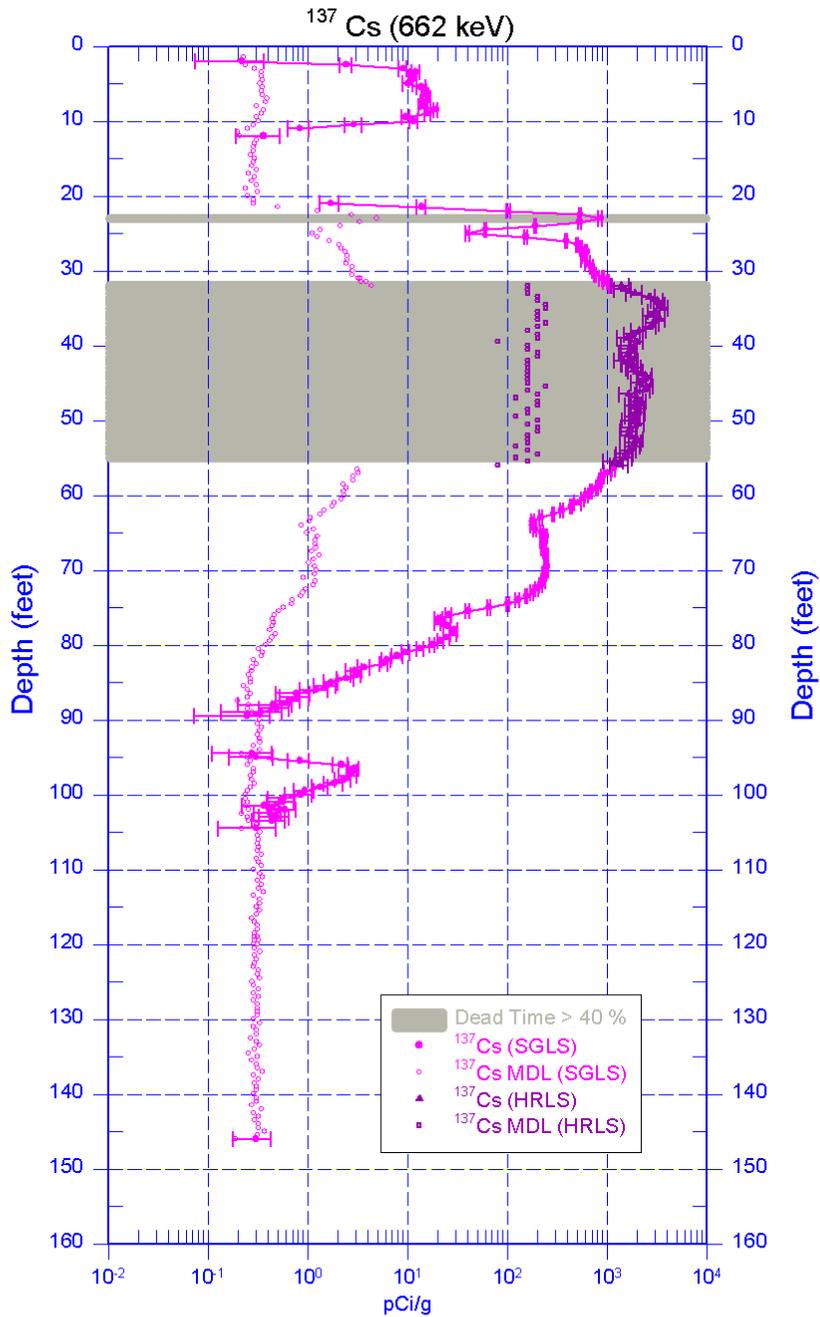


Figure 6-3. A Typical Man-Made Radionuclide Concentration Plot

299-E33-58 (A6866) Combination Plot

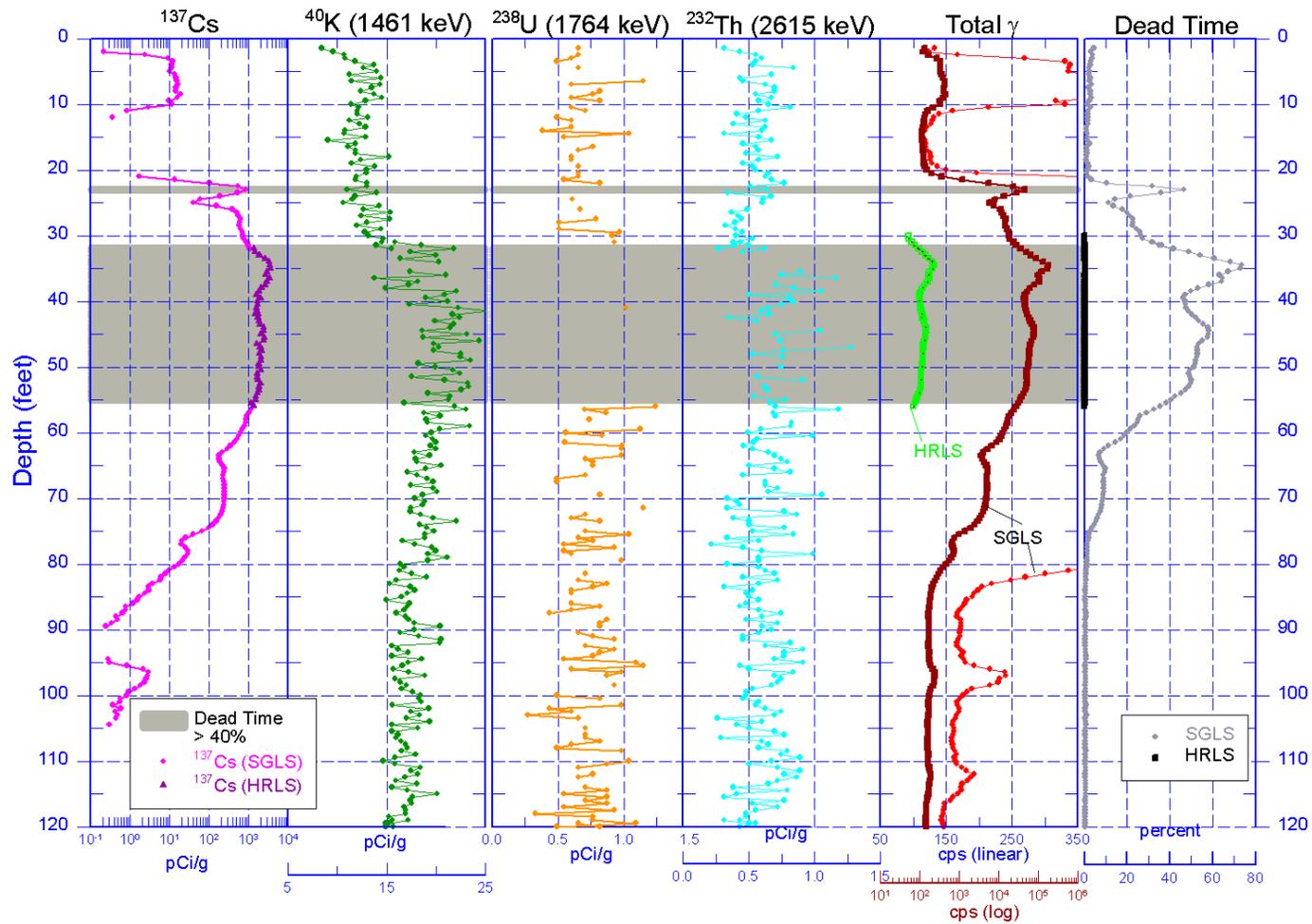


Figure 6-4. A Typical Combination Plot

299-E33-14 (A4841)

Rerun of Natural Gamma Logs

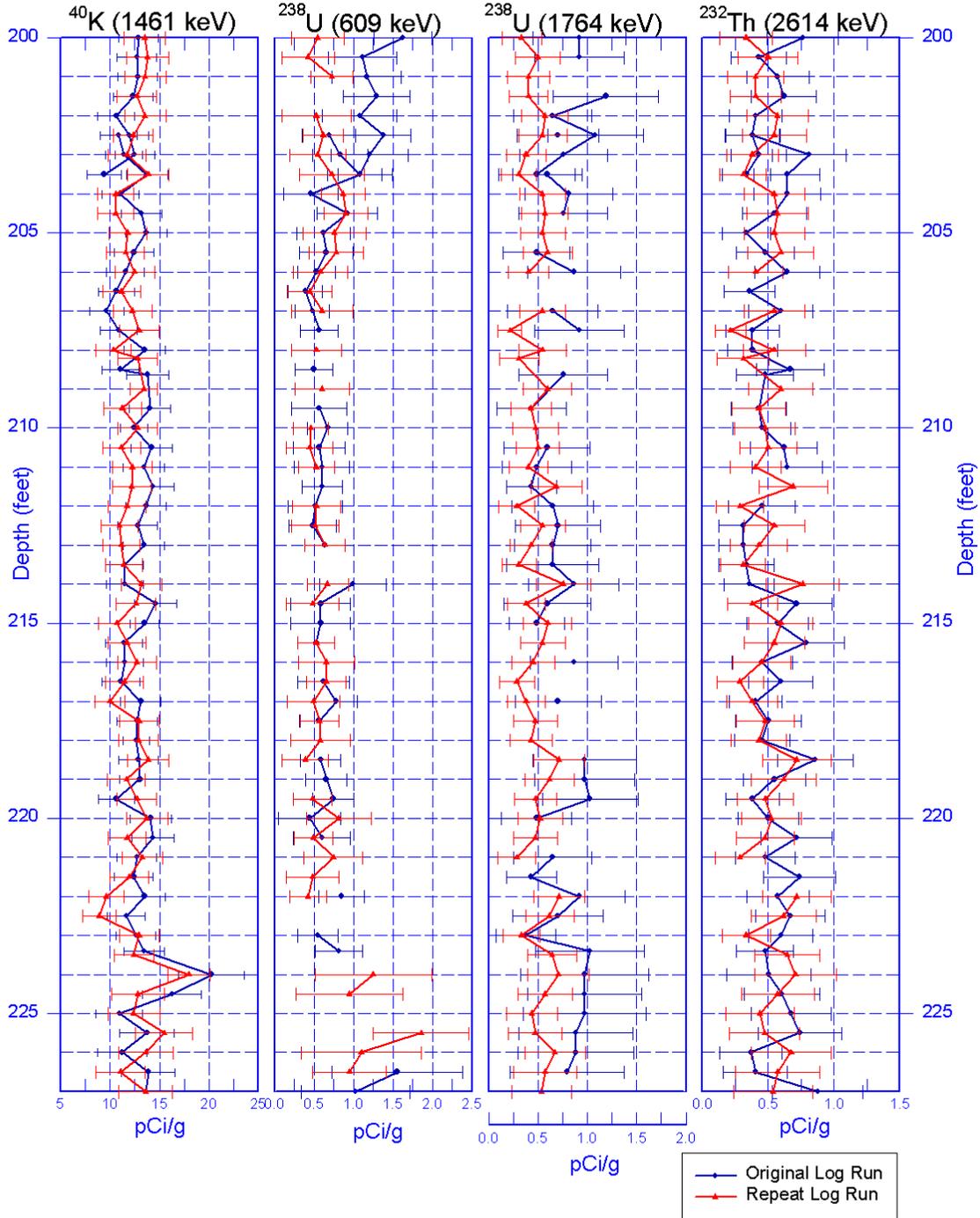


Figure 6-5. A Typical Repeat Plot

The colors, symbols, and line weights shown on the example plots should be considered as guides. Because individual logs and supporting plots may address a wide range of conditions and combinations of contaminants, the analyst is encouraged to use combinations of colors, line weights and symbols that promote readability of the final plot. Although log plots are printed in color, there is a high likelihood that black and white copies will be made by users of the data, and the analyst should endeavor to produce plots that are readable even when copied. Specifically, when two or more plots are shown on the same graph, the analyst should select colors and symbols such that the plots can be distinguished on a black and white copy.

6.2 Log Data Report

The Log Data Report serves as a companion to the log plots and provides supplemental information necessary for log evaluation. The Log Data Report describes borehole conditions and logging operations, including pertinent notes and observations from field personnel, and documents assumptions made during the data analysis process. It also provides a summary of log results and interpretations. The main sections of a Log Data Report with their contents are listed below:

- Borehole Information
 - Well Name (Well ID)
 - Name of nearest waste site
 - Washington State Plane Coordinates in meters (BHI¹ atlas or from HWIS²)
 - Groundwater level measured from the top of casing (TOC) and the date of the measurement
 - Date borehole was drilled
 - TOC elevation in feet (from HWIS)
 - Total depth of the hole relative to the TOC
 - Method of drilling
- Casing Information
 - Casing type (usually either steel welded or threaded)
 - Stickup of casing (feet) from ground surface
 - Outside and inside diameter of the casing
 - Casing thickness (inches)
 - Top and bottom of each casing string
- Borehole Notes
 - Any pertinent borehole information with the source
- Logging Equipment Information
 - Logging System
 - Type
 - Calibration date and reference
 - Logging Procedure

¹ BHI – Bechtel Hanford, Inc.

² HWIS – Hanford Well Information System

- Log Run Information
 - Date, depth range, and file names for each log run
- Logging Operation Notes
 - Any pertinent data and observations related to the logging operation
- Analysis Notes
 - Analyst
 - Date
 - Data Analysis Manual Reference
 - Paragraph discussing the pre-run and post-run verification spectra. Brief discussion of data processing. Reference *Excel* worksheet and calibration date. Include specific reference to the casing thickness and borehole diameter used to calculate casing and water correction factors. (For dual casing, the thickness used is the sum of the individual thickness measurements.)
- Log Plot Notes
- Results and Interpretations
 - Brief description of the distribution of man-made radionuclides
 - Paragraph describing the KUT log and any apparent stratigraphic markers
 - Comparison of the current logging event to any previous logging event(s) (if applicable)
 - Recommendations for additional logging or other investigations
- References

An example Log Data Report is included as Figure 6-6. The Log Data Report is saved as a Microsoft *Word* (*.DOC) file in the working directory for the borehole and accompanies the processed data. The Log Data Report and log plots are printed to an Adobe Acrobat (*.PDF) file, which constitutes the electronic deliverable.

299-E33-41 (A4867) Log Data Report

Borehole Information:

Borehole: 299-E33-41 (A4867)		Site: 216 B-7A and B Crib			
Coordinates (WA St Plane)		GWL¹ (ft): 256.9		GWL Date: 05/02	
North	East	Drill Date	TOC² Elevation	Total Depth (ft)	Type
137369.94 m	573707.19 m	03/91	658.25 ft	263	cable tool

Casing Information:

Casing Type	Stickup (ft)	Outer Diameter (in.)	Inside Diameter (in.)	Thickness (in.)	Top (ft)	Bottom (ft)
stainless steel (ss)	3.43	6.625	6.375	0.125	0	unknown
ss	0.9	N/A ³	4	0.125	0.9	244.9
ss #10 slotted screen	None	N/A	4	0.125	244.9	261.0

Borehole Notes:

The casing depth information provided above is derived from *Summaries of Well Construction Data and Field Observations for Existing 200-East Aggregate Operable Unit Resource Protection Wells* (Ledgerwood 1992). Stoller personnel measured the 6-in. casing wall thickness and the outside diameter; the inside diameter is calculated. The casing thickness is estimated at 0.125 in. for both the 4-in. ID casing and the slotted screen. Groundwater level is derived from Stoller measurements from the top of the 6-in. casing at the time of logging. Coordinates and TOC elevation are derived from HWIS⁴.

Logging Equipment Information:

Logging System: Gamma 1D	Type: SGLS (35%)
Calibration Date: 07/01	Calibration Reference: GJO-2001-243-TAR
Logging Procedure: MAC-HGLP 1.6.5 Rev. 0	

Spectral Gamma Logging System (SGLS) Log Run Information:

Log Run	1	2	3	4 repeat	5
Date	05/28/02	05/29/02	05/30/02	05/30/02	
Logging Engineer	Spatz	Spatz	Spatz	Spatz	
Start Depth	60.0	266.0	170.0	95.0	
Finish Depth	140.0	169.0	139.0	69.0	
Count Time (sec)	200	200	200	200	
Live/Real	R	R	R	R	
Shield (Y/N)	N	N	N	N	
MSA Interval (ft)	1.0	1.0	1.0	1.0	
ft/min	n/a	n/a	n/a	n/a	
Pre-Verification	AD001CAB	AD002CAB	AD003CAB	AD003CAB	

Figure 6-6. Sample Log Data Report

Log Run	1	2	3	4 repeat	5
Start File	AD001000	AD002000	AD003000	A003032	
Finish File	AD001080	AD002097	AD003031	A003058	
Post-Verification	AD001CAA	AD002CAA	AD003CAA	A003CAA	

Logging Operation Notes:

Spectral gamma logging was performed in this borehole during May 2002 on three separate days. Logging measurements are referenced to the top of the 6-in. casing and were started at 60 ft in depth. The interval above 60 ft was not logged because of the relatively large borehole diameter and thick annular grout. Logging began at 60 ft to locate the uranium detected in previous logging events. Data were collected at 1-ft depth increments at 200-s counting times. A data repeat section was collected between 69.0 and 95.0 ft to measure logging system performance.

Analysis Notes:

Analyst:	Henwood	Date:	07/26/02	Reference:	
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Pre-run and post-run verifications of the logging system were performed for each day's log event. The acceptance criteria were met for the verification data. Post-run verifications were used for the energy and resolution calibration necessary to process the data.

A casing correction for 0.125-in.-thick casing is applied for the 5-in. stainless-steel casing and screen. A water correction is applied to data from 257 ft to the total depth of the borehole.

Each spectrum collected during a log run was processed in batch mode using APTEC Supervisor to identify individual energy peaks and determine count rates. Concentrations were calculated with an Excel worksheet template identified as G1DJul01.xls using an efficiency function and corrections for casing, and water as appropriate; no dead time corrections were necessary. The ^{214}Bi peak at 609 keV was used to determine the naturally occurring ^{238}U concentrations rather than the ^{214}Bi peak at 1764 keV. The 609-keV energy peak exhibited slightly better count rates than the 1764-keV peak.

Natural and processed ^{238}U are quantified independently. Natural ^{238}U is assessed from net spectral peak count rates for gamma rays associated with ^{214}Bi , a short-lived decay product of ^{238}U . Typically, the 609- or 1764-keV gamma-ray peaks are used. These assays will yield accurate ^{238}U concentrations only if ^{214}Bi is in secular equilibrium with ^{238}U . Considering the half-lives of the intervening members in the decay chain, a time period on the order of a million years is required for ^{214}Bi to reach secular equilibrium with ^{238}U . Therefore, activity of ^{214}Bi is assumed to be equivalent to natural uranium, which is presumed to have been undisturbed over geologic time. In some cases, this equilibrium may be perturbed by the deposition of ^{214}Bi as a short-term daughter of ^{222}Rn (a highly mobile gas and also a member of the ^{238}U decay series), which may accumulate in boreholes. As the ^{222}Rn dissipates, however, ^{214}Bi activity will decline to levels representative of the ^{238}U concentration in a matter of hours.

Chemical separation and processing of uranium involves the removal of impurities, including the ^{238}U decay products. After uranium has been purified, the longer lived decay products build up very slowly and no gamma activity from ^{214}Bi is detected in processed ^{238}U . Processed ^{238}U is quantified from net count rates for gamma rays (usually 1001 keV) associated with $^{234\text{m}}\text{Pa}$, a short-term decay product that reaches secular equilibrium with ^{238}U within a brief time. The yield of the 1001-keV gamma ray is so low that the spectral peak is undetectable at typical background concentrations.

^{235}U decay is accompanied by emission of a 185.7-keV gamma ray. Because ^{235}U represents only about 0.7% of natural uranium, the overall intensity of this gamma ray in natural uranium is low, and the spectral peak is not observed at typical background concentrations. When ^{235}U is present in anomalous concentrations associated with processed uranium, the 185.7-keV gamma ray can be used for quantification. There is a potential for interference by

Figure 6-6. Sample Log Data Report

the 186.1-keV gamma ray of ^{226}Ra , a long-term decay product of ^{238}U , but the intensity of this gamma ray is generally too weak to affect the ^{235}U assay.

Although ^{235}U and ^{238}U are chemically identical, ^{235}U may have been enriched (or depleted) relative to ^{238}U in processed uranium, and the relative proportions of the two isotopes may be helpful in evaluating the source of the processed uranium.

Log Plot Notes:

Separate log plots are provided for the man-made radionuclides (processed uranium [^{235}U and ^{238}U]) detected in the borehole, naturally occurring radionuclides (^{40}K , ^{238}U , ^{232}Th [KUT]), a combination of man-made, KUT, total gamma and dead time, and a repeat section plot. For each radionuclide, the energy value of the spectral peak used for quantification is indicated. Unless otherwise noted, all radionuclides are plotted in picocuries per gram (pCi/g). The open circles indicate the minimum detectable level (MDL) for each radionuclide. Error bars on each plot represent error associated with counting statistics only and do not include errors associated with the inverse efficiency function, dead time correction, casing corrections, or water corrections. These errors are discussed in the calibration report. A separate log plot is provided that compares the Westinghouse Hanford Company (WHC) Radionuclide Logging System (RLS) data collected in 1991 and 1997 with the current SGLS log data.

Results and Interpretations:

Processed uranium was detected between 78 and 92 ft and from 118 to 243 ft in depth. In the upper interval the maximum ^{238}U concentration measured about 18 pCi/g at 88 ft. In the lower interval the maximum concentrations measured for ^{235}U and ^{238}U were about 35 and 675 pCi/g, respectively, at a depth of 239 ft. Other ^{238}U concentration peaks occur at 123 ft (41 pCi/g), 183 ft (83 pCi/g), 201 ft (116 pCi/g), 223 ft (247 pCi/g), and 230 ft (462 pCi/g). Between 78 and 180 ft in depth, where the measured ^{238}U and ^{235}U concentrations are near their respective MDLs of about 10 and 0.5 pCi/g, both radionuclides may not have been detected at a depth interval. However, both isotopes probably exist where one or the other is detected because they are chemically the same, but one may be just below its MDL.

The KUT concentrations appear to be influenced by the well completion materials and are probably not useful for stratigraphic correlations between boreholes. For example, Ledgerwood (1992) indicates 8-20 mesh bentonite crumbles were emplaced to about 173 ft, where the ^{40}K increases and the ^{238}U and ^{232}Th concentrations decrease. A bentonite slurry was introduced from 173 to 240 ft and bentonite crumbles were emplaced from 240 to 243 ft, where the KUT logs show increases. Below 243 ft a silica sand pack was placed just above and adjacent to the stainless steel screen that was set to 261 ft.

A comparison log plot is included that shows data collected with WHC's RLS in 1991 and 1997 and the SGLS in 2002. The comparison suggests an influx of processed uranium into the area of the borehole from about 155 to 220 ft and increased concentrations between 220 and 240 ft occurred between 1991 and 1997. WHC reported that ^{125}Sb was also detected throughout the borehole in 1991; this radionuclide had decayed away by the second logging event in 1997. The 1991 logging event was conducted before well completion materials had been introduced into the borehole. The SGLS log data show good agreement with the 1997 data and suggest that no movement of contamination has occurred in the area since 1997.

Repeat log sections show good repeatability for depth and radionuclide concentrations, suggesting the logging system was operating properly.

It is recommended repeat logs be collected in this borehole at least twice per year as part of a borehole monitoring program.

Figure 6-6. Sample Log Data Report

References:

Ledgerwood, R.K., 1992. *Summaries of Well Construction Data and Field Observations for Existing 200-East Aggregate Area Operable Unit Resource Protection Wells*, Draft WHC-SD-ER-T12EAA, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

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- ¹ GWL – groundwater level
 - ² TOC – top of casing
 - ³ n/a – not applicable
 - ⁴ HWIS – Hanford Well Information System

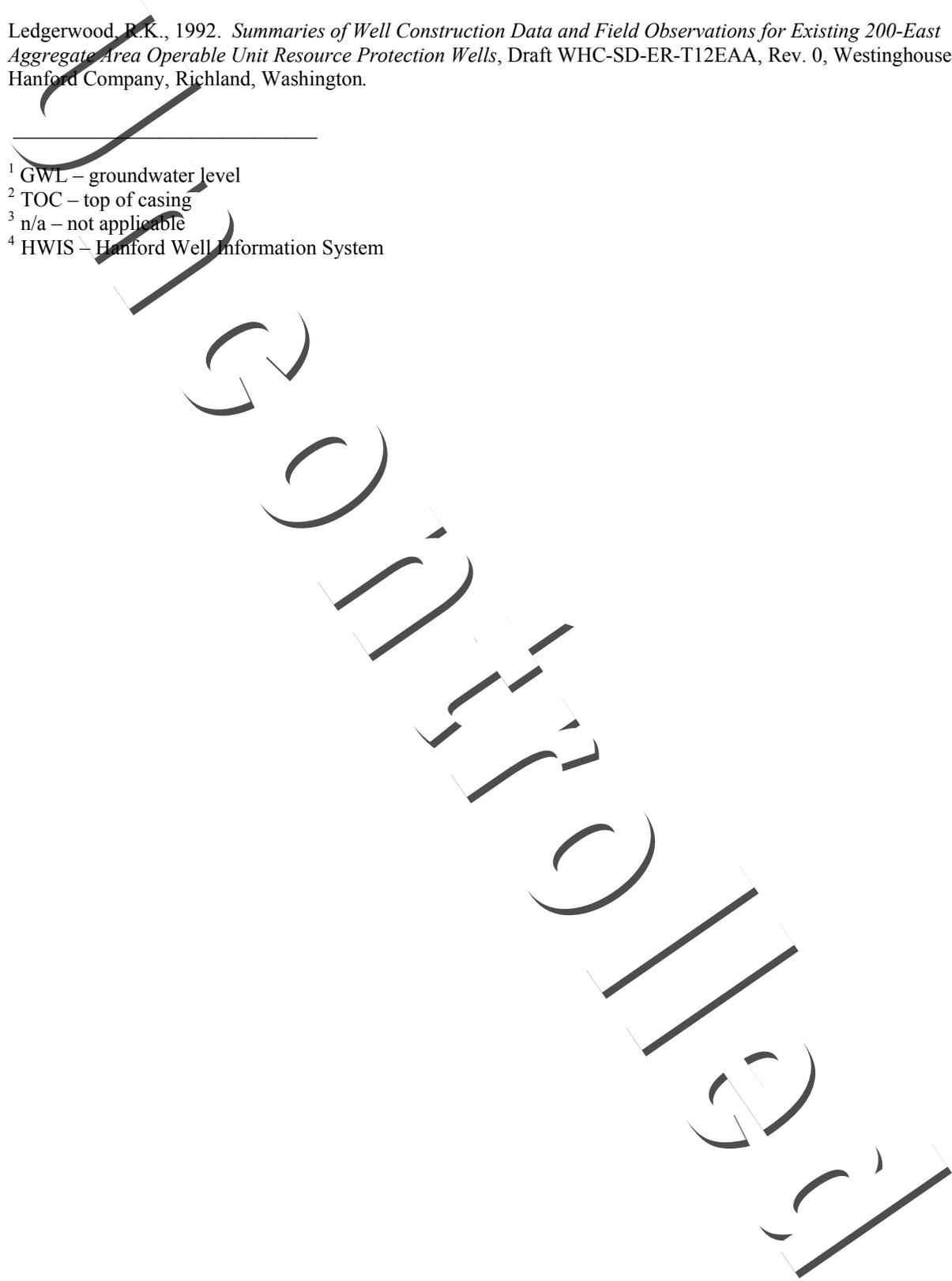


Figure 6-6. Sample Log Data Report

7.0 Preparation of Input Files for Visualization Software

Data visualization, as it is applied to the Hanford 200 Areas Spectral Gamma Vadose Zone Characterization Project, refers to the interpolation of the analyzed contaminant concentration data throughout the three-dimensional space that constitutes the vadose zone at a particular waste site. The visualizations are created as a possible scenario for the distribution and extent of the contaminant plumes and are presented in the waste site reports.

The modeling software used to create the visualizations is *Environmental Visualization System (EVS)* from C Tech Development Corporation. This software incorporates sophisticated three-dimensional variography and kriging under the control of an expert system and a Windows graphical user interface with a three-dimensional graphics application. *EVS* provides total control of generation and rendering of the contaminant plume distribution.

Input for the *EVS* software consists of “chemistry” files (*.CSV), which contain the radionuclide concentration data from the *SigmaPlot* files of interest in the area of investigation. The *EVS* software dictates the format for these chemistry files. Isotopes detected in minimal occurrences are not usually modeled. Several different radionuclides can be contained in a single *.CSV file or each radionuclide can be in a separate file (*.CSV). “Chemistry” files must be in ASCII format. Values within a line can be delimited by commas, spaces, or tabs. They must have a .CSV suffix to be selected in the file browsers of *EVS* modules. The table shown below lists part of a “chemistry” file.

East	North	Depth	185	427	661	1001	1274	1332	1408	BHN	TOC
-1											
3090	7										
1881455	450431.3	2.5	0	0	0.278965	0	0	0	0	E33-21	671.2
1881455	450431.3	3	0	0	0.55793	0	0	0	0	E33-21	671.2
1881455	450431.3	3.5	0	0	1.58855	0	0	0	0	E33-21	671.2
1881455	450431.3	4	0	0	9.833512	0	0	0	0	E33-21	671.2
1881455	450431.3	4.5	0	0	38.28018	0	0	0	0	E33-21	671.2
1881455	450431.3	5.01	0	0	47.92772	0	0	0	0	E33-21	671.2
1881455	450431.3	5.51	0	0	64.48738	0	0	0	0	E33-21	671.2
1881455	450431.3	6.01	0	0	84.2319	0	0	0	0	E33-21	671.2
1881455	450431.3	6.51	0	0	80.43488	0	0	0	0	E33-21	671.2
1881455	450431.3	7	0	0	46.67238	0	0	0	0	E33-21	671.2
1881455	450431.3	7.5	0	0	49.02033	0	0	0	0	E33-21	671.2
1881455	450431.3	8	0	0	51.30629	0	0	0	0	E33-21	671.2
1881455	450431.3	8.5	0	0	60.72911	0	0	0	0	E33-21	671.2
1881455	450431.3	9.01	0	0	104.6118	0	0	0	0	E33-21	671.2
1881455	450431.3	9.51	0	0	209.8436	0	0	0	0	E33-21	671.2
1881455	450431.3	10	0	0	247.58	0	0	0	0	E33-21	671.2
1881455	450431.3	10.5	0	0	486.0253	0	0	0	0	E33-21	671.2
1881455	450431.3	11	0	0	461.7599	0	0	0	0	E33-21	671.2
1881455	450431.3	11.5	0	0	736.9611	0	0	0	0	E33-21	671.2
....											

The first three lines in the file describe the dataset and subsequent lines contain the subsurface data. Line 1 contains header information. Line 2 is a flag to identify the type of Z coordinate system that is used. In the example dataset, -1 or (-1.0) indicates log depths are being used. If elevations are used, then line 2 would contain a 1 or (1.0). The first integer in Line 3 is the number of data points to follow. The second integer on line 3 is the number of radionuclides per depth. Line 4 is the first line of the sample data. Line 4 must follow a set format: x, y, z, values,

borehole name, and reference elevation. Additional details on the *EVS* file formats can be found in the *EVS* reference manuals.

A chemistry file for a cross section or fence diagram has the exact same format, except that the samples from each boring must occur in the order of connectivity along the cross section, and they should be sorted by increasing depth at each sample location.

The radionuclide concentration data that constitute the SGLS and HRLS data plotted in *SigmaPlot* are placed in the "chemistry" file that defined the position in space of each data sample point and the nuclide-specific concentration for that point. These data files are revised to create an "Interpreted Data Set," and the visualizations are based on these revisions. The revisions consist of removing radionuclide concentrations that are not considered to be representative of actual formation concentrations and by averaging the data over a 2.5-ft sample interval. This reduces the total number of data points in the "interpreted data set" and provides a better balance between the vertical and horizontal distributions of data points.

The kriging algorithms in *EVS* use the twenty closest points to estimate concentration. When the data are not averaged, all 20 points are likely to come from the same borehole, because the data density along the borehole axis is much greater than the spatial distribution of boreholes. With fewer data points in each borehole, the kriging algorithm will tend to search over a wider area and is more likely to "find" data in additional boreholes.

This "interpreted data set" reflects interpretations of the distribution and nature of occurrence of the contaminants based on overall experience and familiarity with SGLS logs. The log plots show the distribution of all contamination detected by the logging system, but any values judged to be not representative of in-situ contamination conditions are removed from the interpreted data set. Conditions under which contamination might be removed from the interpreted data set include contamination resulting from dragdown during drilling, contamination on the inside or outside of the casing, and contaminated material that may have accumulated at the bottom of the borehole. Occurrences of ^{137}Cs and ^{60}Co (regardless of the concentrations) generally are not deleted when they appear to be laterally correlatable boreholes, or when they are continuous at depth with no evidence of contamination higher in the borehole. Finally, the edited data set or "interpreted data set" differs from log data in that logging run overlaps are eliminated and SGLS and HRLS data are combined.

Structures depicted in the visualization are rendered within *EVS* from building files. These model files are ASCII files. They must have a *.BLDG suffix to be selected by the *EVS* buildings module file browser. Additional details on the *EVS* buildings can be found in the *EVS* reference manuals.

EVS provides many options for data presentation described in the *EVS* software manual. Retaining the network of *EVS* module in an application file preserves the steps taken in creating a particular visualization. *EVS* application files have a *.V suffix.

EVS provides many options for data presentation described in the *EVS* software manual. Upon completion of a particular visualization in *EVS*, the image is saved as a *.BMP file, normally

with 1280x960 resolution. The *.BMP file is imported into other graphics software such as *Adobe Illustrator*, for annotation. Axes and the depth scale are labeled and north arrow concentration legends, and other notation are added.

After a waste site report has been completed, all pertinent visualizations are archived on CD-ROM with the other data utilized to complete the particular report. In addition, the *.V, *.CSV and *.INF files for the various radionuclides are archived in the event that additional visualizations (e.g., different isolevel, different viewpoint, etc.) are requested.

8.0 Verification Tests of Microsoft® Excel Calculations Used for Log Data Reduction

8.1 Introduction

Associated with a gamma-ray-emitting radionuclide in the subsurface are fluxes of gamma rays with characteristic energies. For example, ^{60}Co is a source of gamma rays with energies 1173.2 keV and 1332.5 keV. If a sufficient number of gamma rays with a characteristic energy impinge upon the gamma-ray detector, the recorded spectrum will have a full energy peak, which represents an elevated count rate at the pulse height corresponding to the characteristic energy. The concentration of the gamma-ray source is proportional to the intensity of the full energy peak.

Spectra are analyzed with a spectrum analysis program named *PCMCA/WIN* (Version 6.3.1, Release 13, Aptec Engineering Ltd.¹, North Tonawanda, New York). With *PCMCA/WIN*, a spectrum is energy-calibrated², then full energy peaks are identified, the associated gamma-ray energies are calculated, and the peak intensities, in counts per second, are calculated. The gamma-ray energy is the basis for the identification of the source radionuclide, and the peak intensity is the basis for the determination of the radionuclide concentration.

If P_n represents the intensity of a full energy peak, in counts per second, the concentration, C_a , of the source radionuclide is calculated by

$$C_a = \frac{27.027}{Y} \times I(E) \times P_n \times K_{DT} \times K_C \times K_W \times K_S \quad \text{Eq. 8-1}$$

Table 8-1 displays descriptions of the symbols and their units.

Table 8-1. Symbols and Units for Quantities Used in Calculations

Symbol	Description	Unit
27.027	conversion factor 27.027 picocuries = 1 decay per second	picocuries per decay per second
Y	gamma-ray yield	gamma rays per decay
$I(E)$	logging system calibration function	(gamma rays per second per gram) per (count per second)
E	gamma-ray energy	kilo-electron-volts ³
P_n	full energy peak intensity	counts per second
K_{DT}	dead time correction	(none)
K_C	correction for the casing in the borehole	(none)
K_W	correction for water in the borehole (if present)	(none)
K_S	correction for shielding (if present)	(none)

¹ Aptec NRC and its subsidiaries merged with Canberra Industries, Incorporated, in January 2002.

² This determines the relationship between pulse height (or MCA channel number) and gamma-ray energy.

³ A kilo-electron-volt is 1,000 electron volts; an electron volt is 1.60×10^{-19} joules.

When the indicated units are used, the radionuclide “concentration” (actually, decay rate per unit mass) is expressed in picocuries⁴ per gram.

Specific $I(E)$ functions have been derived for each logging system. These calibration functions depend on the gamma-ray energy, E . The casing, water, and shield corrections, K_C , K_W , and K_S , are energy-dependent, and in addition, K_C depends on the thickness of the casing and K_W depends on the diameter of the borehole.

The dead time correction, K_{DT} , is independent of the gamma-ray energy, but is a function of the system dead time.

This section of the Data Analysis Manual documents the verification of the calculations used to determine radionuclide concentrations from peak intensity values provided by *PCMCA/WIN*. The verification was performed according to instructions in QA Instruction 6.2, “Computer Program Software Testing,” of the *Grand Junction Office Quality Assurance Manual* (GJO 1).

The verification does not apply to calculations performed by *PCMCA/WIN*.

8.2 Hardware and Software

The concentration calculations, and associated calculations, such as the casing correction determination, are programmed in a Microsoft[®] *Excel* spreadsheet. The following hardware and software were used for the verification demonstration.

Computer

Gateway, system model E-4650, 1794-MHz Intel X86 Family 15 Model 1 processor.
U.S. DOE property number S19473.

Operating System

Microsoft[®] Windows XP Professional, version 5.1.2600.

Spreadsheet Program

Microsoft[®] *Excel* 2000, Product ID 50627-700-1143417-02078.

⁴ A curie is a decay rate of 3.7×10^{10} decays per second; a picocurie is 10^{-12} of a curie.

8.3 Overview of Calculations

8.3.1 Data Acquisition and Processing Overview

This section presents a broad overview of the data acquisition and processing. These topics are discussed in greater depth in other sections of this Data Analysis Manual.

During logging, each spectrum is recorded on the hard disk of the computer that controls logging. When the logging is finished, the spectra are transferred to a transportable medium, such as zip disk. The spectra are then copied onto the office network server and the hard disk in the data analyst's computer.

The analyst uses the *PCMCA/WIN* program to identify full energy peaks and determine the energy, intensity, intensity uncertainty, and minimum detectable activity associated with each peak. An *identify* feature in *PCMCA/WIN* compares the energies to entries in a library energy file to determine the gamma-ray sources. Example 1 displays part of a *PCMCA/WIN* output file for a spectrum named A0069052.S0⁵

⁵ A logging system named Gamma 1D recorded the spectrum while logging the Hanford borehole 299-E33-02 on December 14, 2001.

Example 1. Part of a Typical *PCMCA/WIN* Output File

Aptec *PCMCA/WIN* Spectrum
Aug/27/2002 3:49:20PM

HEADER INFORMATION in A0069052.S0 Imported from Ortec

Identification	Acquisition
User:	Started: Jan/7/1902 1:30:44 PM ⁶
MCARD: 2	Stopped: Jan/7/1902 1:34:04 PM
Detector:	True Time: 200.000 sec
Geometry:	Live Time: 146.540 sec
Sample: 299-E33-2 55.51	Dead Time: 26.73 %
Channels: 4096	Gross Count: 2586432 counts
	Gross Rate: 17650 cps

Sample

Energy Calibration Jan/24/2002 12:58:16PM A0069CAA
Resolution Calibration Jan/24/2002 12:58:47PM A0069CAA.S0
Isotope Library X:\LOGANAL2\SGLS.LIB Aug/30/2001 9:32:30AM

ACTIVITY INFORMATION with MDA's for A0069052.S0 Imported from Ortec

Name	Energy keV	Flag	Activity ⁷ cps	Error cps	MDA ⁸
Cs-37	661.66	m	633.6	± 3.19%	2.350
Eu-154	1274.44	s	0.7085	± 35.69%	0.2448
K-40	1460.83	s	0.9810	± 17.84%	0.1739
Th-232	583.19	*?	-0.08635	± 2000.00%	3.150
Th-232	2614.53	*	0.1290	± 50.84%	0.06442
U-238	609.31	*?	-0.5506	± 2000.00%	3.013
U-238	1764.49	s	0.08642	± 58.96%	0.05330

Errors Quoted at 2 Sigma
MDA's Quoted at 1.645 Sigma

Several simple programs (*Loganal2*, *SGLSoffline*, *RDFCAL*) read the spectral files and the *PCMCA/WIN* output files, organize peak intensity and other data for specific gamma rays, and write a set of output files, one for each gamma ray. Table 8-2 displays data from part of an output file for the 661.6-keV gamma ray of ¹³⁷Cs. These data were extracted from spectra that were recorded by a system named Gamma 1D, while logging the Hanford borehole named 299-E33-02 on December 14, 2001. Note that the last spectrum in Table 8-2 corresponds to the output file in Example 1.

⁶ Acquisition dates are incorrect because the data acquisition program is not Y2K compliant.

⁷ "Activity" is the Aptec Engineering term for peak intensity.

⁸ "MDA" is the minimum detectable activity.

Table 8-2. Example of Compiled Data for the 661.6-keV ¹³⁷Cs Gamma Ray

Spectrum File Name	Depth (feet)	Dead Time (percent)	Peak Intensity (counts per second)	Peak Intensity Uncertainty (percent)
A0069043.S0	46.5	0.64	0.06	186.73
A0069044.S0	47.5	0.45	0.01	2000
A0069045.S0	48.5	0.8	0.05	228.14
A0069046.S0	49.5	1.07	2.27	15.91
A0069047.S0	50.5	8.94	95.71	6.57
A0069048.S0	51.5	31.52	614.1	2.92
A0069049.S0	52.5	30.49	644.8	2.97
A0069050.S0	53.5	25.38	550.2	3.07
A0069051.S0	54.5	25.42	552.8	2.72
A0069052.S0	55.51	26.73	633.6	3.19

Loganal2, *SGLSOffline*, and *RDFCAL* do not perform calculations, they simply retrieve and organize data from spectrum files and *PCMCA/WIN* output files. These programs do not require verification testing. Proper program operation easily is confirmed by comparing the outputs with the *PCMCA/WIN* outputs. For example, the *PCMCA/WIN* output in Example 1 showed an activity (peak intensity) of 633.6 cps \pm 3.19 percent for the peak associated with the 661.6-keV gamma ray of ¹³⁷Cs in spectrum A0069052.S0. This exactly agrees with the corresponding *Loganal2* output for that gamma-ray peak in that spectrum (Table 8-2, last row).

8.3.2 Radionuclide Concentration Calculations

As indicated in Section 8.1, the concentration, C_a , of a radionuclide is calculated with Equation 8-1. This section discusses the various terms in Equation 8-1.

Conversion factor 27.027

This factor is used in the conversion from radioactive decays per second to picocuries. A curie is 3.7×10^{10} decays per second, by definition, and a picocurie is 10^{-12} curies. Therefore, a picocurie is 3.7×10^{-2} decays per second, and a decay per second is $(3.7 \times 10^{-2})^{-1}$ picocuries. Thus, 1 decay per second is equal to 27.027 picocuries.

Gamma-ray yield, Y

Gamma-ray yields, usually expressed in gamma rays per 100 decays, are published in compilations of nuclear data. Data from two publications are used: *Table of Isotopes*, Eighth Edition, Volume I (Firestone 1996), and *Table of Isotopes*, Eighth Edition, Volume II (Firestone 1999). The yield for the 661.6-keV ¹³⁷Cs gamma ray is 85.1 gamma rays per 100 decays (Firestone 1996); for calculations this yield is expressed as 0.851 gamma rays per decay. Yields for commonly encountered gamma peaks associated with naturally occurring and man-made radionuclides are included in Tables 4-4 and 4-5 (Section 4.0).

Calibration function, $I(E)$

DOE (1995) determined that the calibration function can be expressed as

$$I(E) = (A + B \times \ln(E))^2, \quad \text{Eq. 8-2}$$

in which E is the gamma-ray energy, expressed in kilo-electron-volts, and A and B are constants with values particular to the unique combination of sonde and logging system. The logging systems are recalibrated annually, and the recalibrations usually yield slightly revised values for the calibration constants. Values for A and B are provided with individual calibration certificates.

Gamma-ray energy, E

Like gamma-ray yields, energies are published in compilations of nuclear data. Energies published in Firestone (1996) and Firestone (1999) are used. Energy values for commonly encountered gamma peaks associated with naturally occurring and man-made radionuclides are included in Tables 4-4 and 4-5 (Section 4.0).

Dead time correction, K_{DT}

The dead time correction is a function of the dead time, which is determined by the data acquisition system and recorded in the spectrum file and the *PCMCA/WIN* output file (see Example 1). DOE (1995) showed that the dead time correction is equal to 1.0 if the dead time is 10.5 percent or less, and the correction can be expressed as

$$K_{DT} = \frac{1}{F + G \times (DT) \times \ln(DT) + H \times (DT)^3} \quad \text{Eq. 8-3}$$

if the percent dead time exceeds 10.5 percent. DT is the percent dead time and F , G , and H are constants with values particular to the logging system. Given below are values for the logging systems currently in use.

Logging Unit	Range	F	G	H
SGLS Gamma 1A, 1B & 1D	> 10.5 %	1.0080	-4.71 E-4	-5.73 E-7
SGLS Gamma 2A&2B		1.0322	-1.213 E-3	-1.89 E-7
RLS-1	> 18 %	1.03	-4.8 E-4	-4.8 E-7

Casing correction, K_C

Calibration data are recorded “open hole,” (i.e., the instrument is in a test hole without casing or liquid). However, all boreholes at Hanford were constructed with steel casing and the attenuation of gamma rays by casing reduces the spectral peak intensities in relation to the intensities that would have been measured in the absence of casing. Multiplying a peak intensity

by the casing correction (which is always larger than 1) yields a value corresponding to the intensity that would have been recorded if the borehole had no casing.

Koizumi (2002) derived the following equation for the casing correction:

$$K_C = \exp\left(A_C + B_C \times E + \frac{C_C}{E}\right). \quad \text{Eq. 8-4a}$$

In Equation 8-4a, E is the gamma-ray energy, expressed in kilo-electron-volts, and A_C , B_C , and C_C are factors that are linearly related to the wall thickness of the casing. If T is the casing wall thickness, expressed in inches, the thickness-dependent factors are

$$A_C = -0.022 + 1.241 \times T \quad \text{Eq. 8-4b}$$

$$B_C = 1.17 \times 10^{-5} - 0.000213 \times T \quad \text{Eq. 8-4c}$$

$$C_C = 17.2 + 353.2 \times T \quad \text{Eq. 8-4d}$$

(Koizumi 2002).

Water Correction, K_W

Calibration data are recorded without water in the test hole, but boreholes at Hanford may contain water. When the instrument in the borehole is immersed in water, gamma rays from the formation are attenuated and the recorded count rates are lower than would have been the case if water had been absent. Multiplying a peak intensity by the water correction yields a value that corresponds to the intensity that would have been recorded without water.

Koizumi (2002) derived the following equation for the water correction:

$$K_W = \exp\left(A_W + B_W \times E + \frac{C_W}{E}\right). \quad \text{Eq. 8-5a}$$

Equation 8-5a has the same form as Equation 8-4a. E is the gamma-ray energy, expressed in kilo-electron-volts, and A_W , B_W , and C_W are factors that depend on the borehole diameter. (The thickness of the layer of water around the instrument depends on the borehole diameter.)

For this correction to be applicable, the instrument must be centered in the borehole.

If D is the borehole diameter, expressed in inches, the diameter-dependent factors are

$$A_W = \left(1.406 - \frac{4.51}{D}\right)^2 \quad \text{Eq. 8-5b}$$

$$B_W = -0.000307 + \frac{0.00124}{D} \quad \text{Eq. 8-5c}$$

$$C_w = \frac{D}{0.168 - 0.0097 \times D}$$

Eq. 8-5d

(Koizumi 2002).

Shield Correction, K_S

When a zone with extreme concentrations of contaminants is logged, the gamma-ray flux may be so intense that the instrument dead time is excessive, or the system may even be incapable of recording useful spectra.

Under such conditions, useful log data can sometimes be recorded with a tungsten pipe, or shield, installed over the instrument. When data are recorded with the shield installed, a correction K_S ,

$$K_S = \exp\left(A_S + \frac{B_S \times \ln(E) + C_S}{E^2}\right),$$

Eq. 8-6

must be applied to the peak intensities before the radionuclide concentrations are calculated. E is the gamma-ray energy, expressed in kilo-electron-volts, and the parameters A_S , B_S , and C_S have constant values:

$$\begin{aligned} A_S &= (5.888 \pm 0.028) \times 10^{-1} \\ B_S &= (56.9 \pm 1.2) \times 10^3 \\ C_S &= (-31.9 \pm 6.8) \times 10^3. \end{aligned}$$

Since the high rate logging system has been deployed, the shield is rarely used to extend the range of the SGLS, and shield corrections are not included in the *Excel* worksheet. When the shield is used, data will be processed separately.

8.3.3 Uncertainties in Calculated Radionuclide Concentrations

Each calculated radionuclide concentration value is accompanied by an estimate of the experimental uncertainty. When a borehole is logged at different times, the uncertainties help investigators distinguish changes in radionuclide concentrations from concentration variations that are mainly caused by normal fluctuations in full energy peak count rates.

The equation, i.e., Equation 8-1,

$$C_a = \frac{27.027}{Y} \times I(E) \times P_n \times K_{DT} \times K_C \times K_W \times K_S,$$

which is used to calculate the concentration of a radionuclide, was also the basis for the derivation of an expression for the concentration experimental uncertainty. The derivation used

the standard formula for propagation of uncertainties: If F is a function of N independent variables X_1, X_2, \dots, X_N ,

$$F = F(X_1, X_2, \dots, X_N),$$

and if each variable X_N has an uncertainty σX_N , the uncertainty for F is

$$\sigma F = \sqrt{\sum \left(\frac{\partial F}{\partial X_i} \times \sigma X_i \right)^2}.$$

Application of the propagation-of-uncertainties formula to Equation 8-1 yields the following expression for the radionuclide concentration uncertainty:

$$\sigma C_a = C_a \times \sqrt{\left(\frac{\sigma Y}{Y} \right)^2 + \left(\frac{\sigma I(E)}{I(E)} \right)^2 + \left(\frac{\sigma P_n}{P_n} \right)^2 + \left(\frac{\sigma K_{DT}}{K_{DT}} \right)^2 + \left(\frac{\sigma K_C}{K_C} \right)^2 + \left(\frac{\sigma K_W}{K_W} \right)^2 + \left(\frac{\sigma K_S}{K_S} \right)^2}.$$

All of the terms on the right side of the above equation, except one, are discarded on the following grounds.

The gamma-ray yield uncertainty, σY , is a *systematic* uncertainty; for a particular gamma ray the uncertainty assumes a constant value.

The uncertainties in the shield, casing, and water corrections, σK_S , σK_C , and σK_W , are also systematic uncertainties; their values for a particular gamma ray energy do not change as long as the casing thickness and borehole diameter remain unchanged.

For a specific energy, the uncertainty in the calibration function, $\sigma I(E)$ is also a systematic uncertainty.

The uncertainty in the dead time correction is also a systematic uncertainty.

Thus, for the assessment of the signals due to a particular gamma ray in a particular borehole, the sum of the six systematic uncertainties is a term that increases the relative concentration uncertainties by a constant amount. This consistent increase in the uncertainties is unhelpful for monitoring purposes (i.e., when a borehole is periodically re-logged to interrogate for concentration changes) because the larger uncertainties make it harder to distinguish a change in concentration from a statistical fluctuation. For this reason, the systematic uncertainties are left out of the uncertainty determinations.

In summary, the expression for the concentration uncertainty is simplified to

$$\sigma C_a = C_a \times \sqrt{\left(\frac{\sigma P_n}{P_n}\right)^2} = C_a \times \frac{\sigma P_n}{P_n}. \quad \text{Eq. 8-7}$$

The uncertainty for P_n is calculated by *PCMCA/WIN*, using formulas based on the statistics of radioactive decay (Poisson statistics). Verification of these calculations is not included in this report because *PCMCA/WIN* is a commercial program.

8.3.4 Minimum Detectable Level

The minimum detectable level (MDL) is the lowest concentration (activity) of a specific radionuclide for which detection is statistically defensible. *PCMCA/WIN* calculates minimum detectable activity (MDA), based on the background count level in the spectral region of interest. The MDL is calculated using Equation 8-1, and substituting the MDA for the peak count rate. Verification of the MDA calculation is not included because *PCMCA/WIN* is a commercial program.

8.4 Verification Test Details

8.4.1 Calibration Function

Figure 8-1 shows part of the “worksheet”⁹ in the *Excel* file where values of $I(E)$ are calculated. The name of the worksheet is $I(E)$, as indicated on the “tab” at the bottom of the worksheet (below column D). The calibration function $I(E)$ is shown (see Equation 8-2), and values of the calibration constants, A and B , for the particular logging system appear in cells D13 and D14. (The A and B values can be replaced easily after each system recalibration.)

⁹ This is the Excel term for a section of the file that has 16,777,216 cells arranged in 65536 rows and 256 columns.

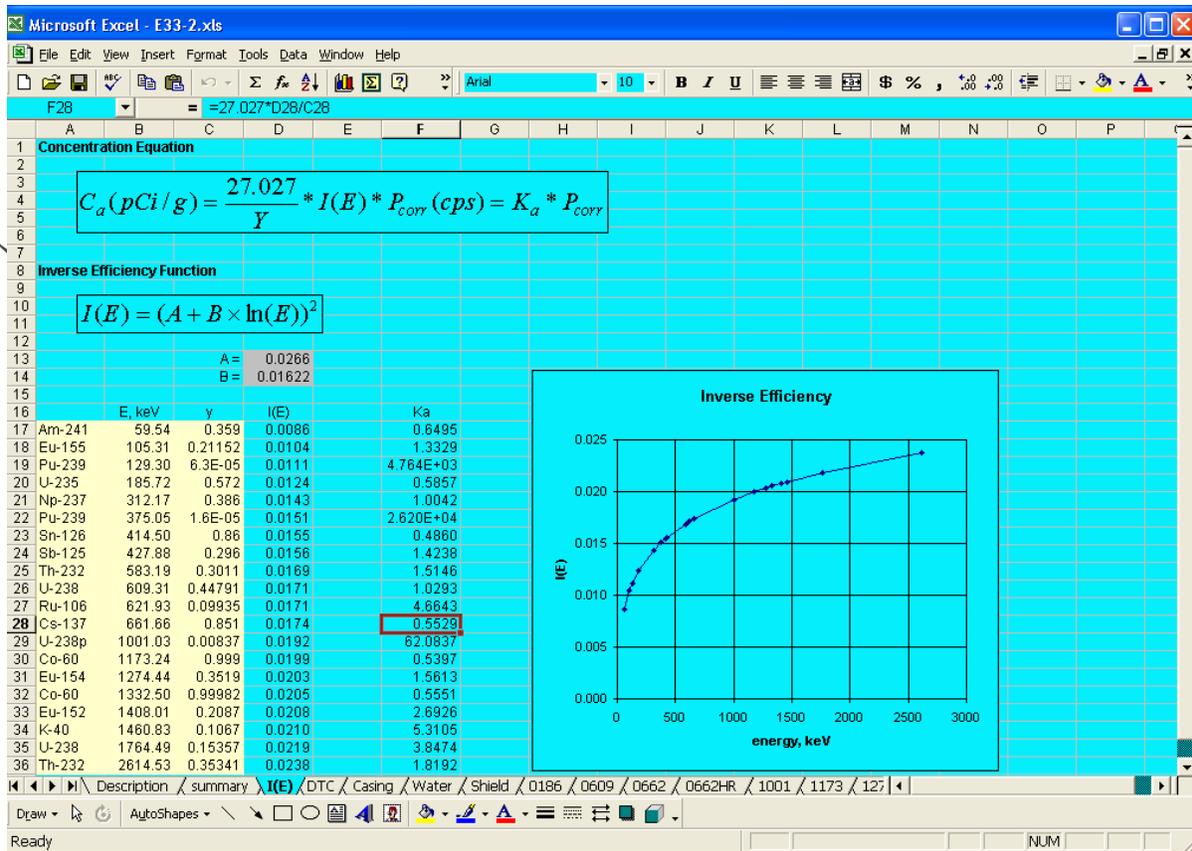


Figure 8-1. Excel Worksheet for Calculations Involving $I(E)$. (Because no calculations are performed in the “Description” and “summary” worksheets, those worksheets are not displayed or discussed.)

The number in the highlighted cell D28 is the value for $I(E)$ for the energy 661.66 keV in cell B28. (The source for this gamma ray is ^{137}Cs , the most commonly encountered gamma-ray-emitting contaminant at Hanford.) The $I(E)$ value is calculated using the formula displayed in the “Formula Bar”¹⁰:

$$=(D\$13 + D\$14*\ln(B28))^2,$$

which is the *Excel* code for

$$(D\$13 + D\$14 \times \ln(B28))^2,$$

which is the right side of Equation 8-2.

$D\$13$ is the entry in cell D13 (calibration constant A), $D\$14$ is the entry in cell D14 (calibration constant B), and $\ln(B28)$ is the logarithm of the energy value in cell B28. The dollar signs, as in $D\$13$, specify *Excel* absolute references; the element following the dollar sign remains fixed when a formula is copied to a number of cells. Thus, when the worksheet was created, the

¹⁰ This line near the top of the worksheet has an “=” immediately to the left. Shown in this line is the number, text, or formula embedded in the associated worksheet cell.

formula was coded in cell D17, then copied to cells D18 through D36. The argument of the log term (that is, the gamma-ray energy) changed from B17 to B18, B19, ... , B36, but the calibration constants in cells D13 and D14 were used in every calculation.

The formula embedded in cell D28 is verified as follows:

$$\begin{aligned} (D\$13 + D\$14 \times \ln(B28))^2 &= (0.0266 + 0.01622 \times \ln(661.66))^2 \\ &= (0.0266 + 0.01622 \times 6.49475)^2 = (0.0266 + 0.10534)^2 \\ &= (0.13194)^2 = 0.0174 = \text{the number in cell D28.} \end{aligned}$$

These verification calculations, and the others that follow, were performed with a Hewlett-Packard HP 11C RPN Scientific Calculator.

As mentioned, the formulas in cells D17 through D36 are identical, except for the $\ln(B_N)^{11}$ term. It is unnecessary to verify each of the entries in these cells.

Figure 8-2 is the same as Figure 8-1, except the K_a value for the energy 661.66 keV (cell F28) is highlighted and the Formula Bar displays the formula used to calculate the K_a value that appears in cell F28.

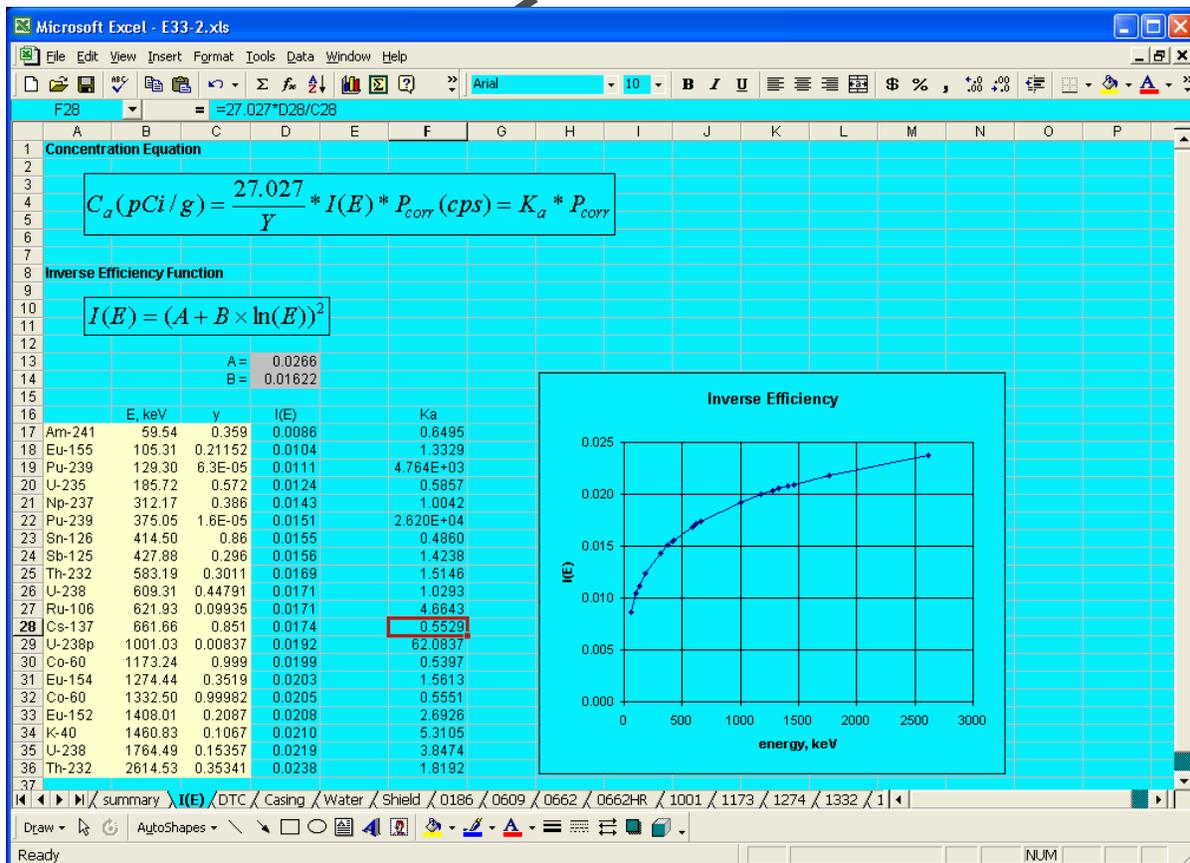


Figure 8-2. Calculation of the K_a Value

¹¹ B_N denotes the cell in column B, row N.

The “Concentration Equation” printed on the worksheet in Figure 8-2 indicates that

$$K_a = 27.027 \times \frac{I(E)}{Y}; \quad \text{Eq. 8-8}$$

this corresponds to the entry in the Formula Bar for cell F28:

$$=27.027*D28/C28.$$

Verification of the calculation for K_a :

$$27.027 * D28 / C28 = 27.027 \times 0.01741 / 0.851 = 0.55293 \approx 0.5529 = \text{the number in cell F28.}$$

The value of 0.01741 for $I(E)$ was used instead of the rounded value of 0.0174 that appears in cell D17. Cells D17 through D36 have been formatted to display numbers with four digits following the decimal, but the *Excel* calculations use the actual values, not the rounded values.

When the worksheet was created, the formula in cell F28 was actually coded in cell F17, then copied to cells F18 through F36. Consequently, cells F17 through F36 have the same formula as cell F28 and it is unnecessary to verify the calculations that yielded the numbers in the cells F_N other than cell F28.

8.4.2 Dead Time Correction

Figure 8-3 shows a Dead Time Correction worksheet. The dead time correction function is identical to Equation 8-3, and the values of the constants, F , G , and H , are displayed in cells B7, B8, and B9.

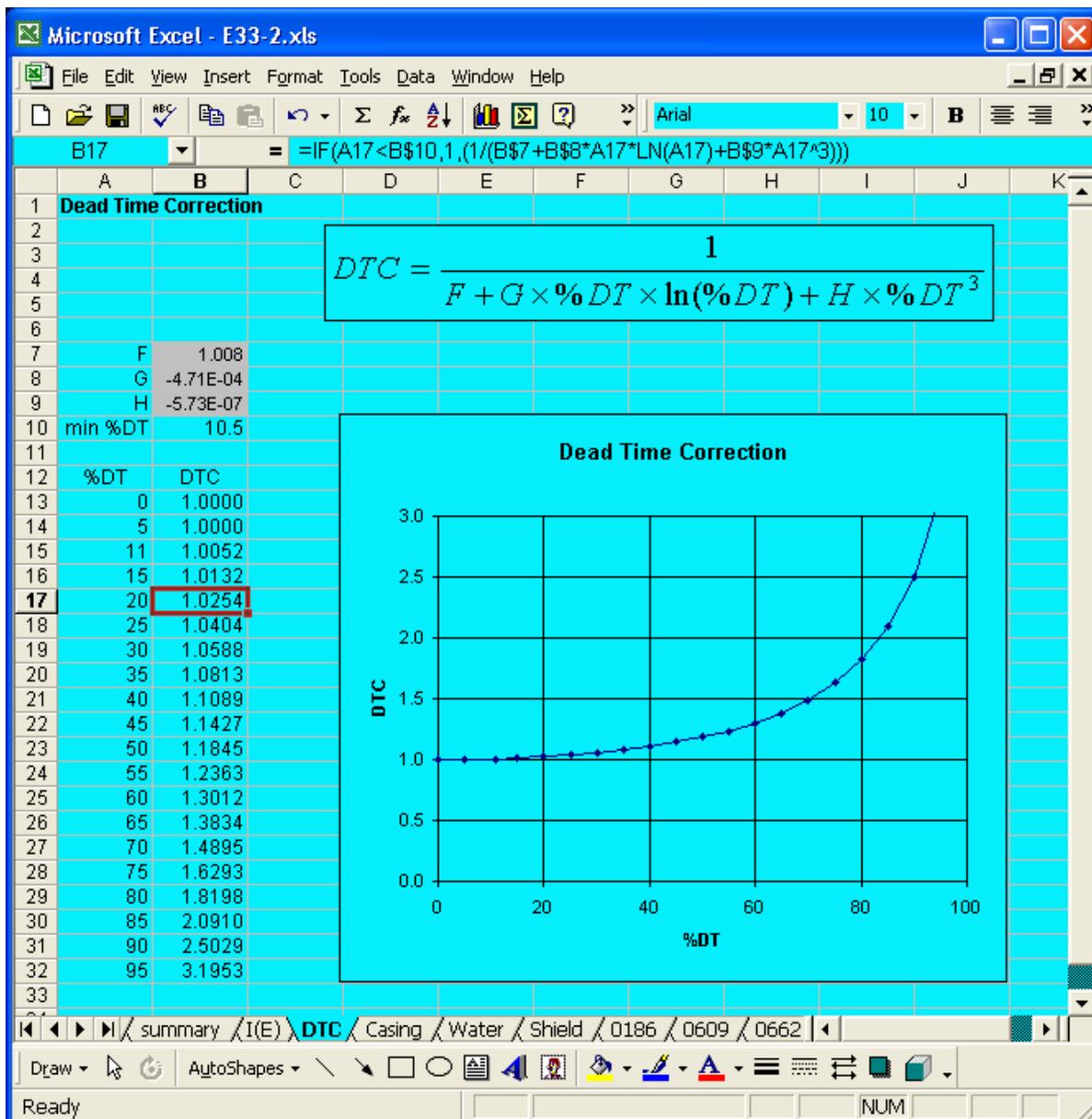


Figure 8-3. Dead Time Correction Worksheet

Cells A13 through A32 contain sample percent dead times, and cells B13 through B32 display the corresponding calculated dead time corrections.

The calculated dead time correction in cell B17 (highlighted) serves for the calculation verification.

The worksheet formula bar indicates that the calculation embedded in cell B17 is

$$=IF(A17<B$10,1,(1/(B$7+B$8*A17*LN(A17)+B$9*A17^3))).$$

According to this formula, the number in cell B17 will be 1.0 if $A17 < B\$10$, (i.e., the dead time correction is unity if the percent dead time is less than 10.5, as mentioned in Section 8.3.2). If the percent dead time is greater than 10.5, the correction is

$$1/(B\$7+B\$8*A17*LN(A17)+B\$9*A17^3),$$

or

$$\frac{1}{F + G \times (DT) \times \ln(DT) + H \times (DT)^3}$$

as specified by Equation 8-3.

Since $A17 = 20$, which is greater than 10.5, the number in cell B17 is

$$\begin{aligned} 1/(B\$7+B\$8*A17*LN(A17)+B\$9*A17^3) &= 1/(1.008 - 4.71 \times 10^{-4} \times 20 \times \ln(20) - 5.73 \times 10^{-7} \times (20)^3) \\ &= 1/(1.008 - 4.71 \times 10^{-4} \times 2.99573 - 5.73 \times 10^{-7} \times (8000)) = 1/(1.008 - 0.02822 - 0.00458) \\ &= 1/0.97520 = 1.02543 \approx 1.0254 = \text{the number in cell B17.} \end{aligned}$$

It is also worth noting that the percent dead times in cells A13 and A14 are less than 10.5, and the corresponding dead time corrections in cells B13 and B14 are equal to 1.0, as required.

Figure 8-4 depicts a worksheet with examples of dead time corrections for borehole data. (This worksheet is for the 661.6-keV gamma ray of ^{137}Cs .) The worksheet row 178 indicates that for the spectrum from the depth of 53.01 ft, the 661.6-keV gamma-ray peak intensity was 648.8 cps (cell C178), the dead time was 28.02 percent (cell B178), and the dead time correction was 1.05 (cell J178).

Depth	deadtime	cps	cpsUnc	mda	flag	filename	cps error	DTC	Kc	Kw	Ks	depth adj	0662d	0662
174	192	0.37	0.12	112.33	0.23	A0067097.LST	0.135	1.00	2.537	1	1	1.402	192.0	#N/A
175	50.01	3.49	21.16	8.52	0.41	A0068000.LST	1.803	1.00	2.537	1	1	1.402	50.0	29
176	51.01	21.28	325.1	4.51	1.8	A0068001.LST	14.662	1.03	2.537	1	1	1.443	51.0	468
177	52.01	37.69	909.5	4.35	2.84	A0068002.LST	39.563	1.10	2.537	1	1	1.536	52.0	1397
178	53.01	28.02	648.8	2.62	2.14	A0068003.LST	16.999	1.05	2.537	1	1	1.474	53.0	958
179	54.01	24.44	506.5	3.12	1.99	A0068004.LST	15.803	1.04	2.537	1	1	1.457	54.0	734
180	55.01	25.56	576	3.84	1.75	A0068005.LST	22.118	1.04	2.537	1	1	1.462	55.0	844
181	56.01	30.12	806.6	3.26	2.38	A0068006.LST	26.295	1.06	2.537	1	1	1.486	56.0	1198
182	57.01	24.52	616.6	3.35	1.79	A0068007.LST	20.656	1.04	2.537	1	1	1.457	57.0	898
183	58.01	22.56	544.3	3.21	2.04	A0068008.LST	17.472	1.03	2.537	1	1	1.448	58.0	788
184	59.01	33.17	863.3	2.99	3.04	A0068009.LST	25.813	1.07	2.537	1	1	1.504	59.0	1298
185	60.01	30.59	816.9	2.82	2.81	A0068010.LST	23.037	1.06	2.537	1	1	1.488	60.0	1214
186	61.01	22.42	570.2	2.35	1.89	A0068011.LST	13.400	1.03	2.537	1	1	1.448	61.0	824
187	62.01	18.82	474.2	3.03	1.46	A0068012.LST	14.368	1.02	2.537	1	1	1.434	62.0	674

Figure 8-4. Dead Time Correction Examples

The formula bar indicates that the dead time correction in cell J178 was calculated as

$$=IF(B178<10.5,1,1/(DTC!B7+DTC!B8*B178*LN(B178)+DTC!B9*B178^3)),$$

or, as

$$1/(DTC!\$B\$7+DTC!\$B\$8*B178*LN(B178)+DTC!\$B\$9*B178^3),$$

because the entry in cell B178 is not less than 10.5. Note that the exclamation point, as in DTC!\\$B\\$8, indicates that the label preceding “!” (DTC in this case) is the name of a worksheet. Thus, DTC!\\$B\\$8 signifies the entry in cell B8 of the DTC worksheet. The designated cells in the DTC worksheet are shown in Figure 8-3.

Verification of the calculation of the number in cell J178 of worksheet 0662:

$$\begin{aligned} & 1/(DTC!\$B\$7+DTC!\$B\$8*B178*LN(B178)+DTC!\$B\$9*B178^3) \\ & = 1/(1.008 - 4.71 \times 10^{-4} \times 28.02 \times \ln(28.02) - 5.73 \times 10^{-7} \times (28.02)^3) \\ & = 1/(1.008 - 4.71 \times 10^{-4} \times 28.02 \times 3.33292 - 5.73 \times 10^{-7} \times 21999.1) = 1/(1.008 - 0.04399 - 0.01261) \\ & = 1/(0.95140) = 1.0511 \approx 1.05 = \text{the number in cell J178.} \end{aligned}$$

Since the formula embedded in cell J178 was copied into all of the dead time correction cells in column J, verification of the calculations for the other cells is unnecessary. It is worthwhile to note that whenever the dead time is less than 10.5 percent, for example, in cells B173, B174, and B175, the corresponding dead time corrections are equal to 1.0, as in cells J173, J174, and J175.

8.4.3 Casing Correction

Part of the casing correction worksheet is depicted in Figure 8-5. At the right side of the figure, a plot of casing correction values in relation to gamma-ray energy is truncated. The missing part of the plot is of no consequence to verification because the plot has no role in the casing correction calculations.

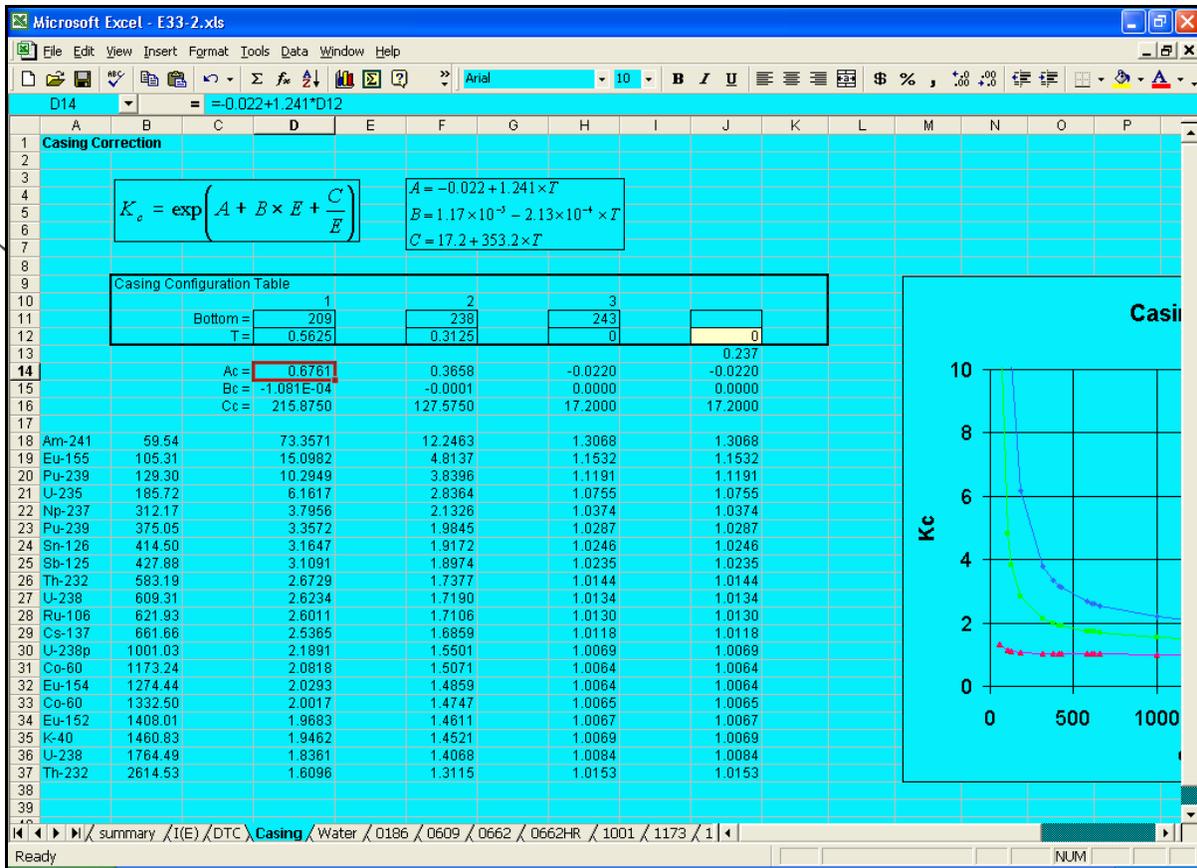


Figure 8-5. Worksheet for Casing Corrections, Showing Calculation of the A_C Factor

The formula for the casing correction is identical to Equation 8-4a, and the factors, A , B , and C (called A_C , B_C , and C_C in Equations 8-4b, 8-4c, and 8-4d) are related to the casing wall thickness, T , expressed in inches, as indicated by Equations 8-4b, 8-4c, and 8-4d.

The three columns D, F, and H, accommodate up to three different casing thicknesses in a borehole. Column J allows calculation of K_c for a fourth casing thickness. This is not used for concentration calculations, but may be useful for comparison purposes. The depths corresponding to the bottoms of casings with particular thicknesses appear in cells D11, F11, and H11 in the “Casing Configuration Table.” The borehole for which this worksheet was prepared had two casing thicknesses: from 209 ft to 238 ft, the thickness was $T = 0.3125$ in. (cell F12), and from 0 to 209 ft, the thickness was $T = 0.5825$ in. (cell D12).

Programs to calculate the values for A_C , B_C , and C_C that correspond to the various casing wall thicknesses are embedded in the cells in columns D, F, H, and J, and rows 14, 15, and 16. Cells in the same columns, but in rows 18 and below, have programs to calculate the casing correction values for the gamma-ray energies in column B.

For example, cell D14 (highlighted in Figure 8-5) shows the calculated value for A_C . The Formula Bar indicates that the value was calculated by

$$=-0.022+1.241*D12,$$

which corresponds to Equation 8-4b. Cell D12 displays the casing thickness, in inches. The calculation of the value in cell D14 is verified as follows:

$$-0.022 + 1.241 \times D12 = -0.022 + 1.241 \times 0.5625 = -0.022 + 0.6981 = 0.6761 \approx \text{the value in cell D14.}$$

In Figure 8-6 the highlighted cell D15 has the programmed calculation

$$=0.0000117-0.000213*D12,$$

which corresponds to Equation 8-4c.

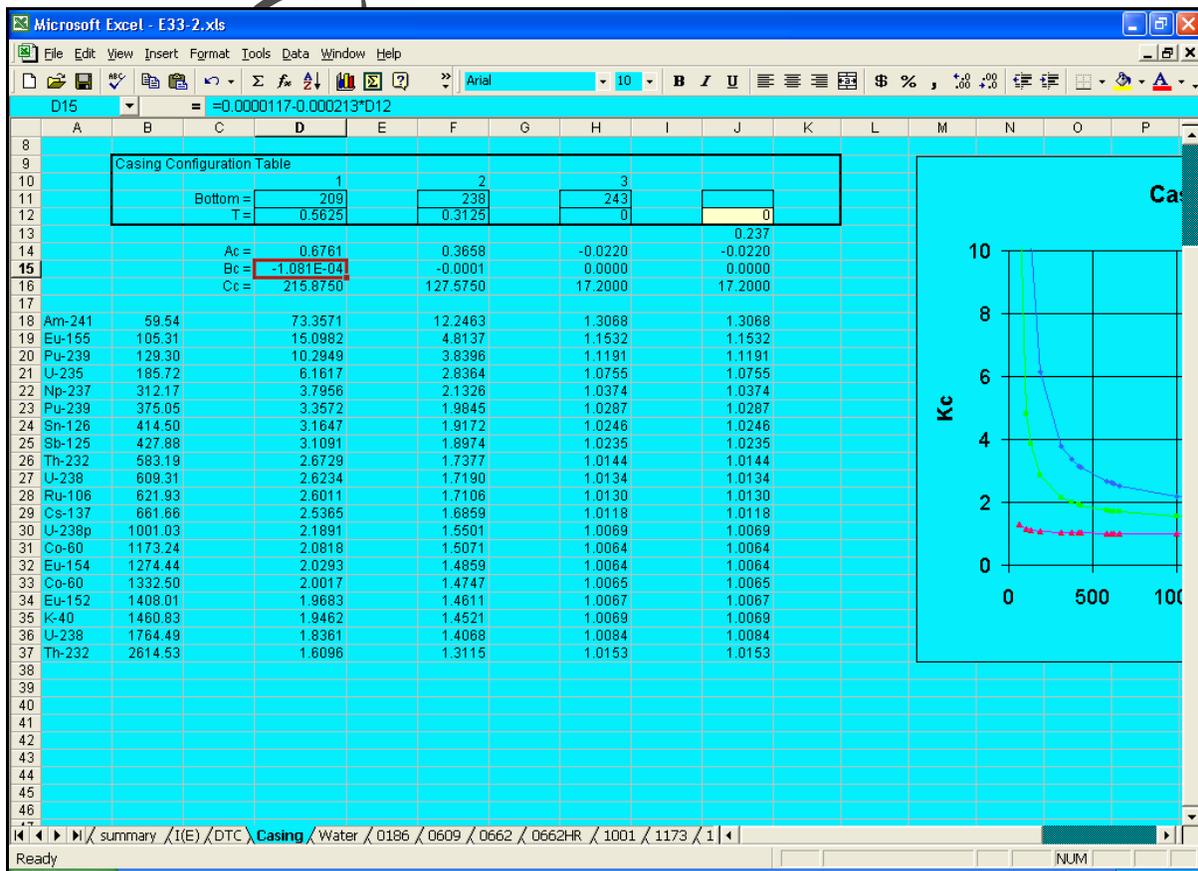


Figure 8-6. Calculation of the B_c Factor in the Casing Correction

The calculation of the value in cell D15 is verified as follows:

$$0.0000117 - 0.000213 \times D12 = 0.0000117 - 0.000213 \times 0.5625 = 0.0000117 - 0.000120 = -0.0001081 \approx \text{the value in cell D15.}$$

In Figure 8-7, the highlighted cell D16 has the programmed calculation

$$=17.2+353.2*D12,$$

which corresponds to Equation 8-4d.

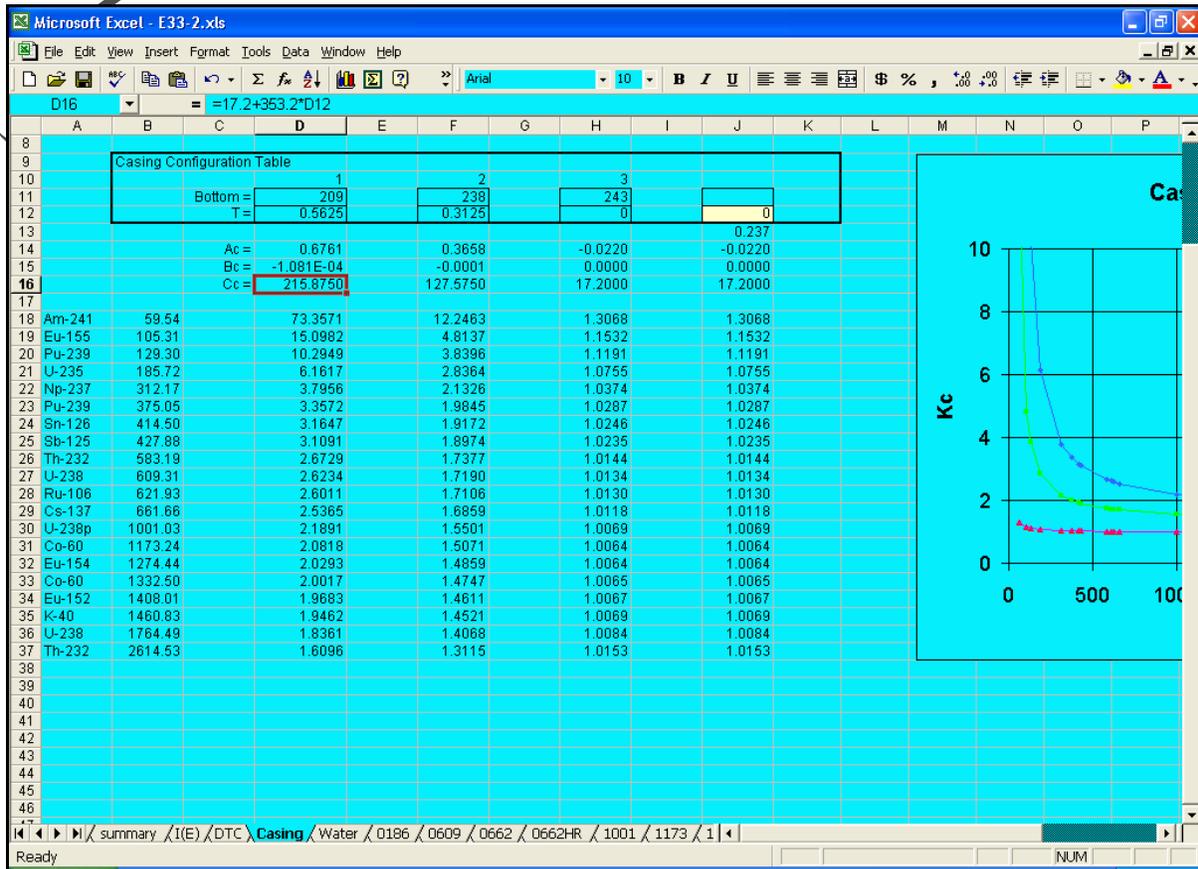


Figure 8-7. Calculation of the C_C Factor in the Casing Correction

The calculation of the value in cell D16 is verified as follows:

$$17.2 + 353.2 * D12 = 17.2 + 353.2 \times 0.5625 = 17.2 + 198.675 = 215.875 \approx \text{the value in cell D16.}$$

The calculations programmed in cells F14, F15, and F16, and H14, H15, and H16, and J14, J15, and J16 are identical to those programmed in cells D14, D15, and D16, except for the thicknesses that are used. The calculations for cells F14, F15, and F16 use the thickness in cell F12, the calculations for cells H14, H15, and H16 use the thickness in cell H12, and the calculations for cells J14, J15, and J16 use the thickness in cell J12.

The actual casing correction values, K_C , for the thickness in cell D12 are calculated in cells D18, D19, and the other cells below D19 in column D. The correction in a particular cell D_N is for the gamma-ray energy displayed in cell B_N . The program for the casing correction in cell D29 is shown in the Formula Bar in Figure 8-8.

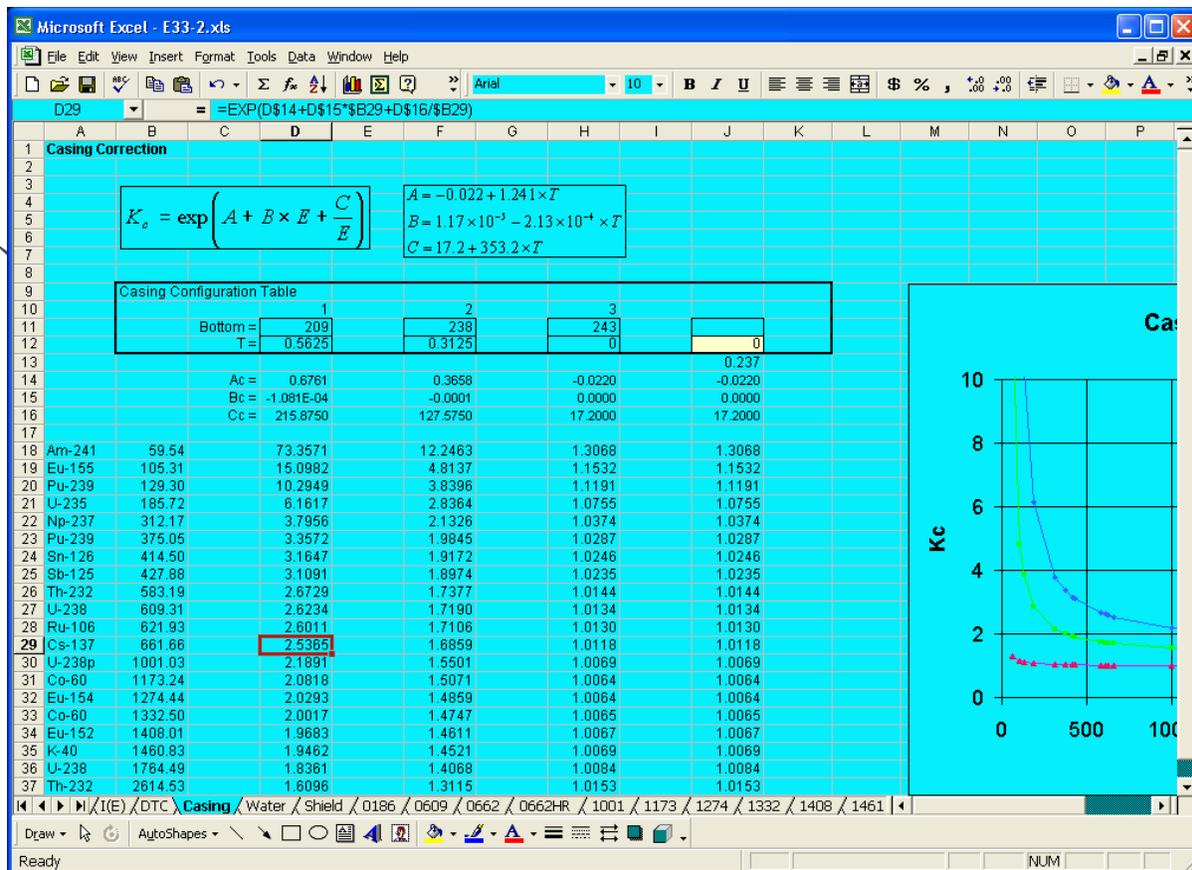


Figure 8-8. Example of Casing Correction Calculation

This calculation,

$$=EXP(D\$14+D\$15*\$B29+D\$16/\$B29),$$

is as specified by Equation 8-4a. The calculation is verified as follows:

$$\begin{aligned} EXP(D\$14+D\$15*\$B29+D\$16/\$B29) &= \exp(0.6761 - 1.081 \times 10^{-4} \times 661.66 + 215.875/661.66) \\ &= \exp(0.6761 - 0.07153 + 0.32626) = \exp(0.93083) \\ &= 2.5366 \approx 2.5365 = \text{entry in cell D29.} \end{aligned}$$

The correction values in cells D18, D19, and the other cells in column D below D19, are calculated by the same method. The same method is also used to calculate the correction values in cells F18, F19, F20, and the other cells below F20 in column F.

The sample spreadsheet illustrated in Figures 5-5 through 5-8 pertains to a borehole with two casing thicknesses, for which the corrections are calculated in the cells in columns D and F. If a borehole has three casing thicknesses, the additional correction can be calculated and displayed in the cells in column H, which are programmed similarly to the cells in columns D and F. Column J is available to calculate correction factors for a fourth casing thickness. In the sample spreadsheet, the thickness entries in cells H12 and J12 are zero, indicating that the cells in columns H and J are not utilized. $T = 0$ cannot be misinterpreted as a borehole configuration

because there are no uncased boreholes at Hanford. Obviously, the casing correction should be unity if $T = 0$. The calculated corrections in columns H and J are not equal to one because the casing correction equation is not exactly correct. The equation was derived using data and curve fitting, and therefore produces approximations to the true corrections.

8.4.4 Water Corrections

Figure 8-9 displays the sample worksheet for the water correction calculations. As indicated in Section 8.3.2, the energy-dependent water correction is calculated with Equation 8-5a (which is also displayed on the sample worksheet). Equations 8-5b, 8-5c, and 8-5d are used to calculate values for the borehole-diameter-dependent factors, A_w , B_w , and C_w .

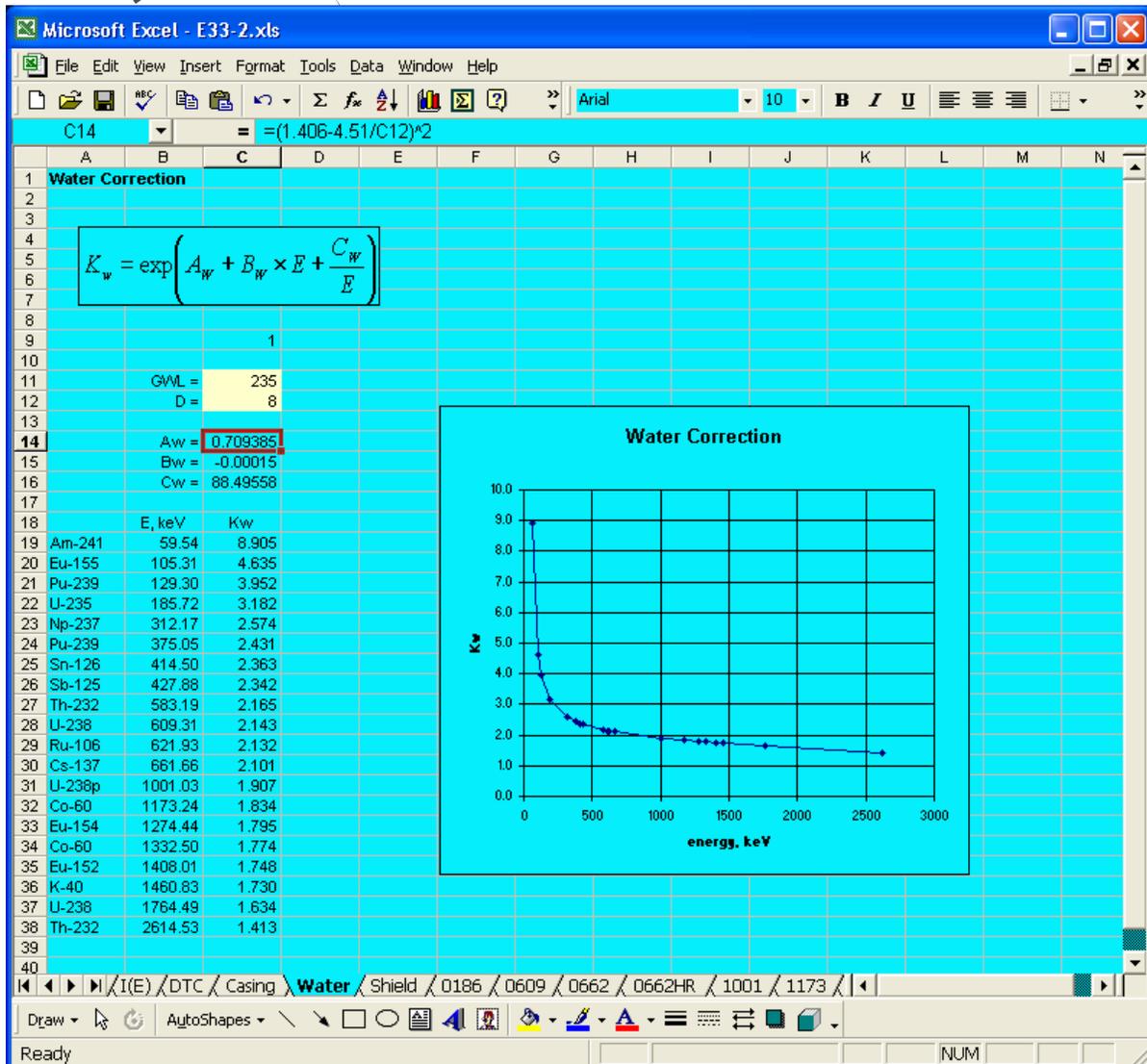


Figure 8-9. Worksheet for Calculating Water Corrections

The depth to water, 235 ft in the example, is shown in cell C11. Cell C12 shows the borehole diameter, 8 in, in this case. The diameter is a factor in the calculation of the value for the A_W factor, as indicated in Equation 8-5b and the Formula Bar for the highlighted cell C14:

$$=(1.406-4.51/C13)^2.$$

Verification of calculation for A_W :

$$(1.406 - 4.51/C12)^2 = (1.406 - 4.51/8)^2 = (1.406 - 0.56375)^2 = (0.84225)^2 = 0.70939 \approx \text{the value in cell C14.}$$

In Figure 8-10, cell C15 with the calculation of the value for B_W is highlighted.

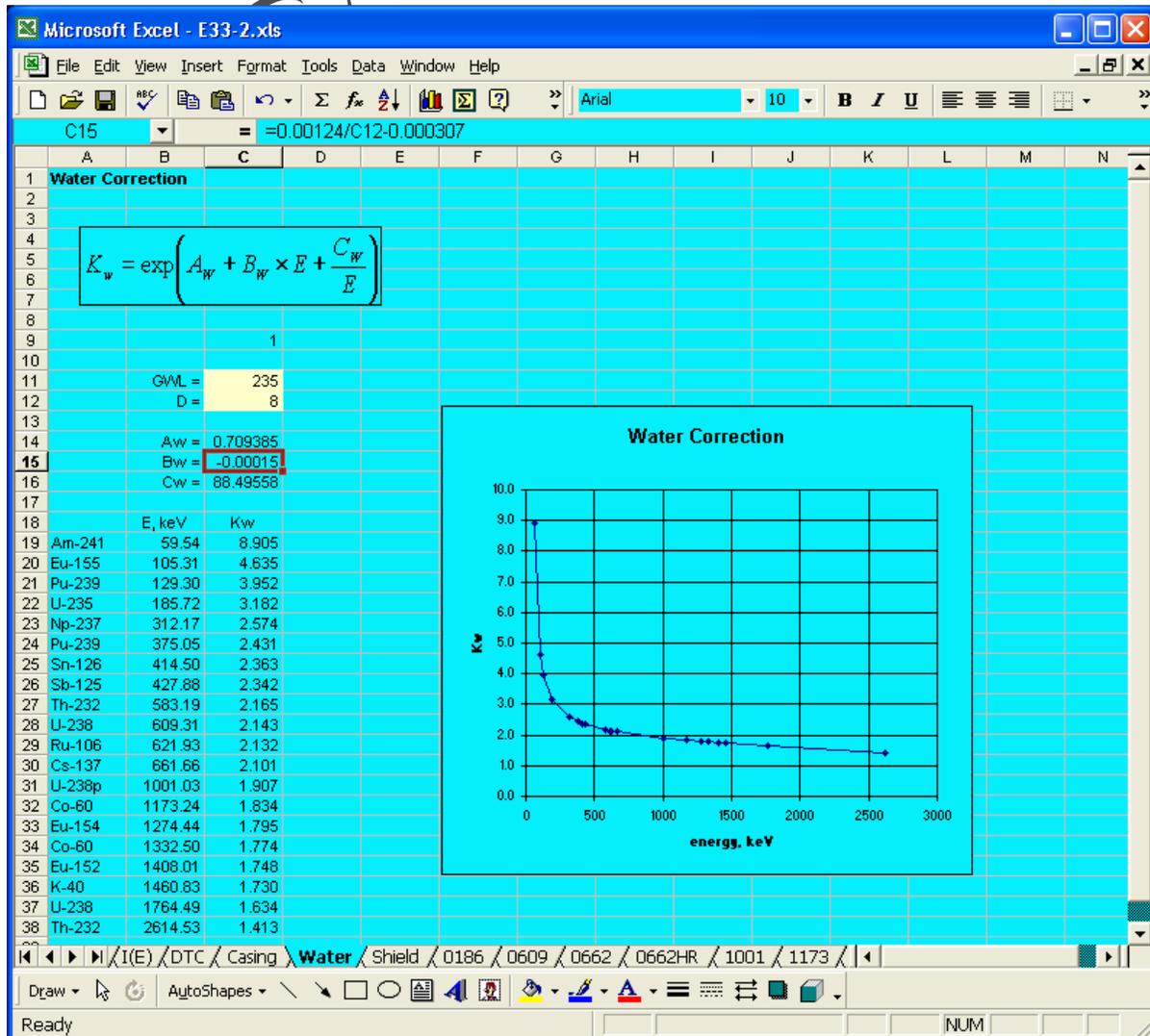


Figure 8-10. Calculation of the B_W Factor in the Water Correction

According to the Formula Bar and Equation 8-5c,

$$=0.00124/C12-0.000307$$

is the formula for the B_W value.

Verification of the calculation of the B_W value:

$$0.00124/C12-0.000307 = 0.00124/8 - 0.000307 = 0.000155 - 0.000307 \\ = -0.000152 \approx -0.00015 = \text{the value in cell C15.}$$

In Figure 8-11, cell C16 with the calculated value for C_W is highlighted. The formula for C_W is

$$=C12/(0.168-0.0097*C12)$$

according to the Formula Bar and Equation 8-5d.

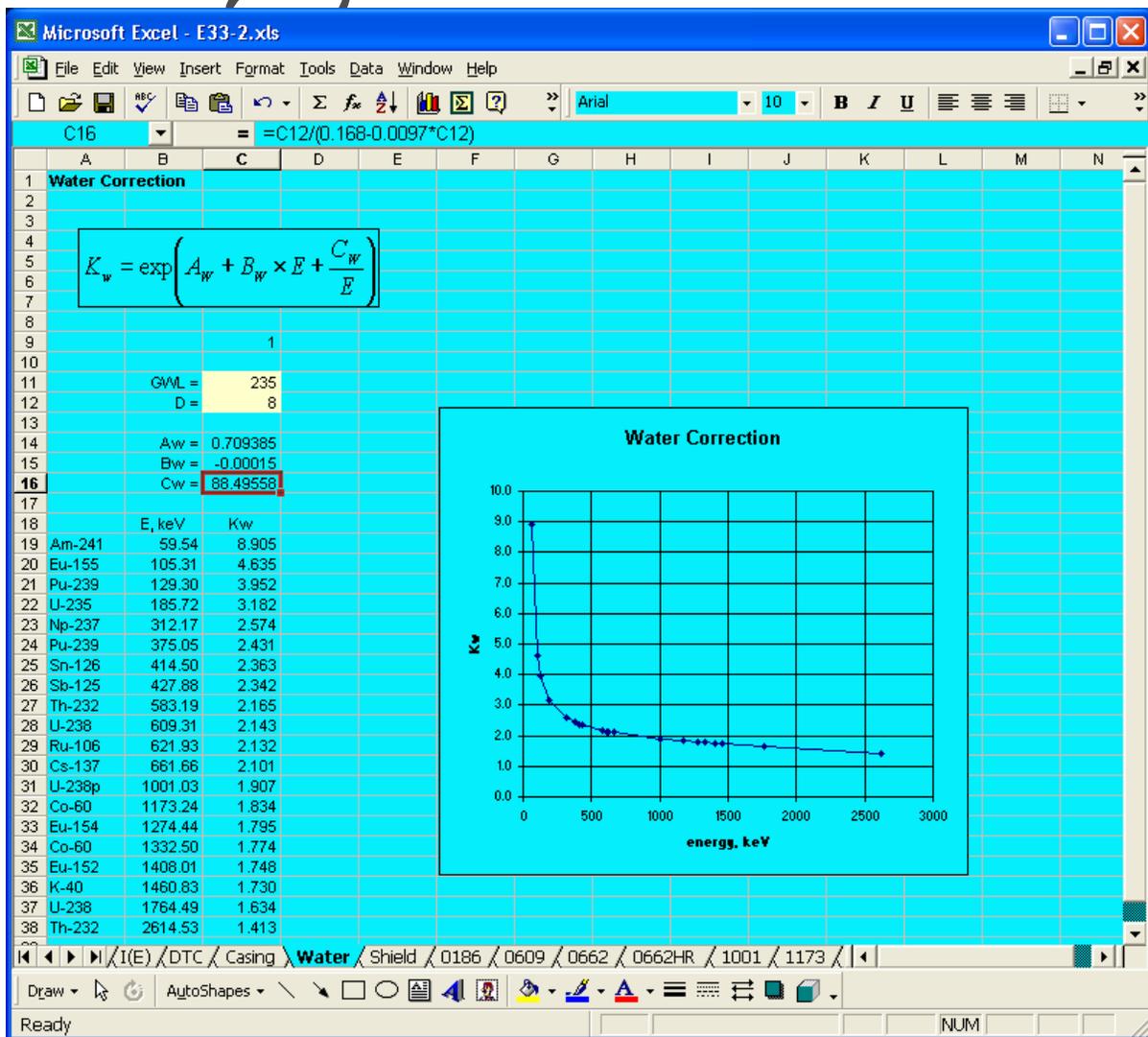


Figure 8-11. Calculation of the C_W Factor in the Water Correction

Verification of the calculation of the C_W value:

$$C12/(0.168-0.0097*C12) = 8/(0.168 - 0.0097 \times 8) = 8/(0.168 - 0.0776) = 8/0.0904 = 88.4956 \approx 88.4956 = \text{the value in cell C16.}$$

The calculated water correction for the gamma-ray energy 661.66 keV (^{137}Cs) resides in cell C30 (highlighted) in Figure 8-12. As indicated by the Formula Bar and Equation 8-5a, the value for K_W is calculated by

$$=EXP(C\$14+C\$15*B30+C16/B30).$$

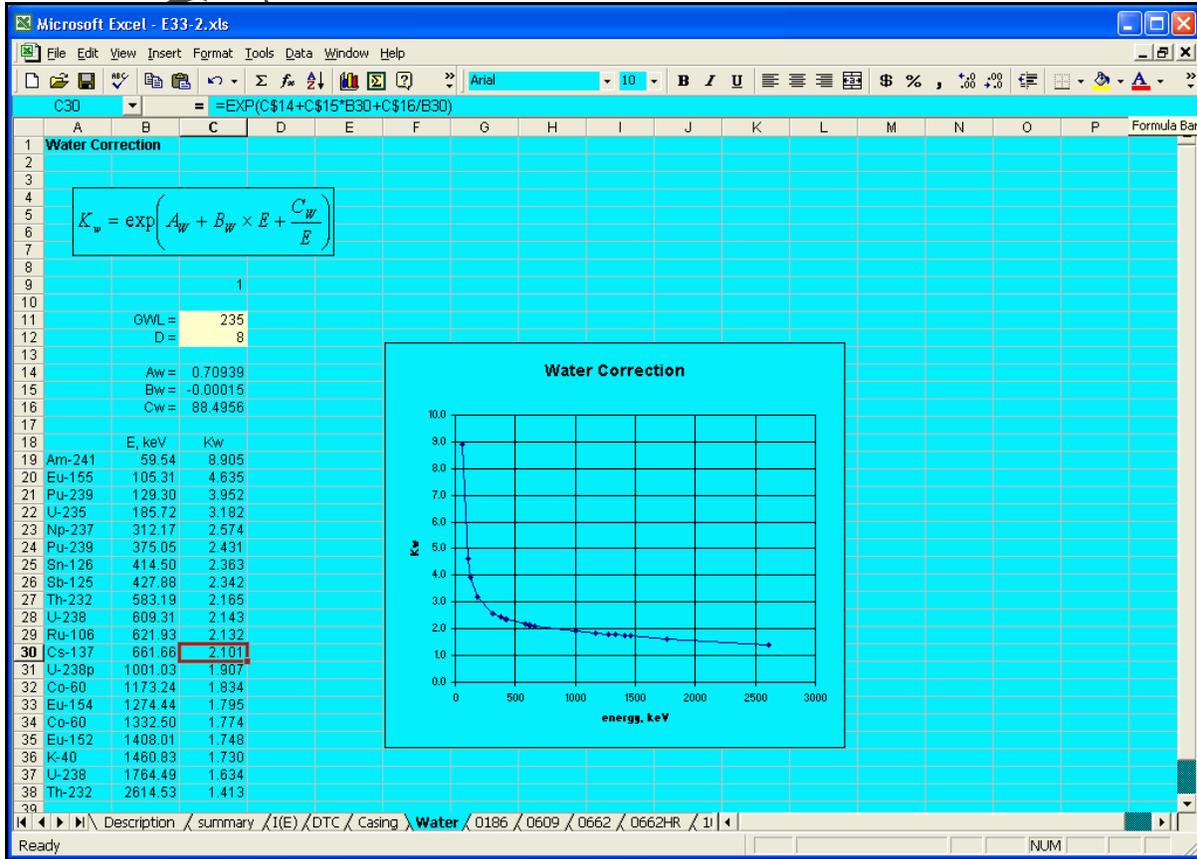


Figure 8-12. Calculation of the Water Correction for the ^{137}Cs Gamma Ray

Verification of the calculation of the K_W value:

$$\begin{aligned} EXP(C\$14+C\$15*B30+C16/B30) &= \exp(0.70939 - 0.000152 \times 661.66 + 88.4956/661.66) \\ &= \exp(0.70939 - 0.1005723 + 0.1337478) = \exp(0.7425655) \\ &= 2.1013 \approx 2.101 = \text{the value in cell C30.} \end{aligned}$$

The other cells in the group, C19 through C38, are programmed similarly to cell C30.

8.4.5 Shield Corrections

Figure 8-13 shows a worksheet for tungsten shield corrections. The shield correction for a particular gamma-ray energy E is calculated with Equation 8-6. The factors A_S , B_S , and C_S have

constant values, as indicated in Section 8.3.2. The three values are also displayed on the worksheet.

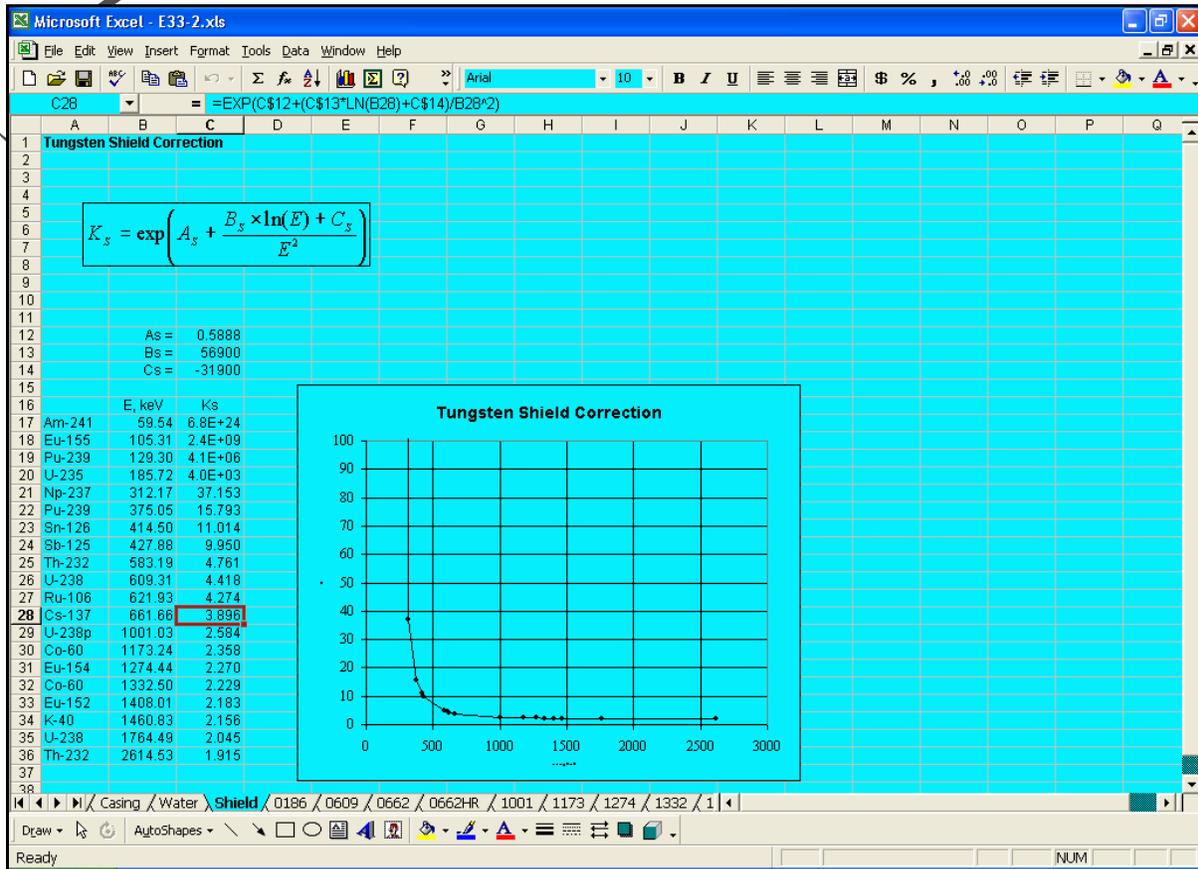


Figure 8-13. Worksheet for Calculation of the Tungsten Shield Correction

The highlighted cell C28 shows the shield correction value for the gamma-ray energy in cell B28, i.e., 661.66 keV (¹³⁷Cs source). The Formula Bar indicates that the code for the calculation is

$$=EXP(C\$12+(C\$13*LN(B28)+C\$14)/B28^2),$$

which is identical to Equation 8-6.

Verification of the K_S value:

$$\begin{aligned} EXP(C\$12+(C\$13*LN(B28)+C\$14)/B28^2) &= \exp(C\$12 + (C\$13 \times \ln(B28) + C\$14)/B28^2) \\ &= \exp(0.5888 + (56900 \times \ln(661.66) - 31900)/661.66^2) \\ &= \exp(0.5888 + (56900 \times 6.494752 - 31900)/437793.96) \\ &= \exp(0.5888 + 337651.389/437793.96) = \exp(1.36006) \\ &= 3.896 \approx 3.896 = \text{the value in cell C28.} \end{aligned}$$

The other cells in the group, C17 through C36, are programmed similarly.

With the availability of the high rate logging system, the tungsten shield is seldom used with the SGLS. Therefore, SGLS calculation worksheets generally do not include provisions for the shield correction. When the shield is used, the data are processed separately from unshielded data, and the shield correction is applied as an additional multiplier to all concentration values.

8.4.6 Radionuclide Concentration Calculations

8.4.6.1 Concentrations

For concentration calculations, there is a worksheet for each gamma-ray energy of interest. Figure 8-14 shows part of the worksheet for the 661.66-keV gamma ray of ^{137}Cs . The energy is recorded in cell I1.

As indicated in Section 8.3.1, a simple program reads the spectral data files and compiles data for each gamma-ray energy. In Figure 8-14, these data appear in rows 5 and beyond, in columns A (depth), B (percent dead time), C (peak intensity in counts per second), D (percent peak intensity uncertainty), E (minimum detectable activity), F (flag), and G (spectrum file name).

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	E:\stan	Log_Data\200EIE33	2logls					661.66	209	2.537	Kw	Ks	Ka		depth adj	
2	Processed	by LogAnal2 V1.0a	T	hu Jan 24	16:04	7:30 2002			238	1.686	235	3.896	0.553		0.0	pC
3									243	1.012	2.101	N			d	a
4	Depth	deadtime	cps	cpsUnc	mda	flag	filename	cps error	DTC	Kc	Kw	Ks		0662d	066	
5	238.00	0.44	0.05	356.68	0.28	??	A0066000.LST	0.178	1.00	1.686	2.10131	1	1.959		238.0	#N
6	237.00	0.49	0.09	161.16	0.25	??	A0066001.LST	0.145	1.00	1.686	2.10131	1	1.959		237.0	#N
7	236.00	0.49	0.06	229.66	0.25	??	A0066002.LST	0.138	1.00	1.686	2.10131	1	1.959		236.0	#N
8	235.00	0.31	0.01	882.92	0.22	??	A0066003.LST	0.088	1.00	1.686	2.10131	1	1.959		235.0	#N
9	234.00	0.35	0.06	247.15	0.25	??	A0066004.LST	0.148	1.00	1.686	1	1	0.932		234.0	#N
10	233.00	0.39	-0.03	2000	0.28	??	A0066005.LST	-0.600	1.00	1.686	1	1	0.932		233.0	#N
11	232.00	0.6	-0.02	2000	0.31	??	A0066006.LST	-0.400	1.00	1.686	1	1	0.932		232.0	#N
12	231.00	0.88	-0.03	2000	0.42	??	A0066007.LST	-0.600	1.00	1.686	1	1	0.932		231.0	#N
13	230.00	0.96	0	2000	0.46	??	A0066008.LST	0.000	1.00	1.686	1	1	0.932		230.0	#N
14	229.00	0.81	0.27	91.33	0.4	??	A0066009.LST	0.247	1.00	1.686	1	1	0.932		229.0	#N
15	228.00	0.59	0.24	81.92	0.32	??	A0066010.LST	0.197	1.00	1.686	1	1	0.932		228.0	#N
16	227.00	0.49	-0.01	2000	0.31	??	A0066011.LST	-0.200	1.00	1.686	1	1	0.932		227.0	#N
17	226.00	0.42	0.11	164.04	0.3	??	A0066012.LST	0.180	1.00	1.686	1	1	0.932		226.0	#N
18	225.00	0.38	0.05	256.83	0.23	??	A0066013.LST	0.128	1.00	1.686	1	1	0.932		225.0	#N
19	224.00	0.24	0.1	22.67	0.12	??	A0066014.LST	0.260	1.00	1.686	1	1	0.932		224.0	#N

Figure 8-14. Part of the Worksheet for the ^{137}Cs Concentration Calculations

Cells J1, J2, J3, K1, K2, and K3 are programmed to retrieve values from other worksheets in this spreadsheet file.

Cell J1

program code: =summary!C4
 action: Copies the entry in cell C4 of the "Summary" worksheet to cell J1.
 description of value: Depth, in feet, corresponding to the bottom of the first casing.

Cell J2

program code: =summary!C5
 action: Copies the entry in cell C5 of the "Summary" worksheet to cell J2.
 description of value: Depth, in feet, corresponding to the bottom of the second casing.

Cell J3

program code: =summary!C6
 action: Copies the entry in cell C6 of the "Summary" worksheet to cell J3.
 description of value: Depth, in feet, corresponding to the bottom of the third casing, (also the total depth of the borehole).

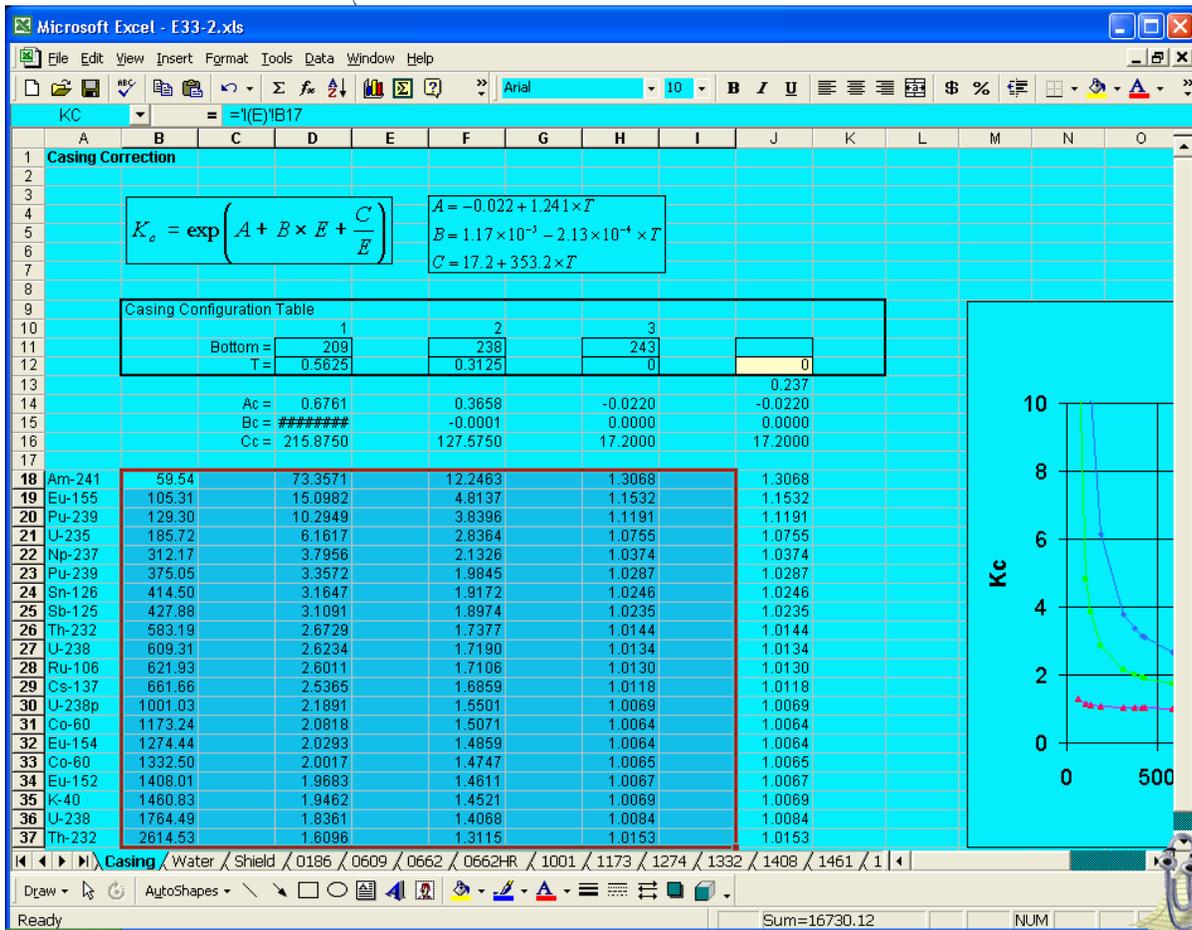


Figure 8-15. The "KC" Block of Cells in the Casing Correction Worksheet

Cell K1

program code: `=VLOOKUP(I1, KC,3)`
action: Copies to cell K1 the value in column 3 of the row that contains \$I\$1 (=661.66) in the range "KC" which is defined as *Casing*\$B\$18:\$I\$37 (i.e., the rectangular block of cells in the "Casing" worksheet with cells B18 and I37 at the corners). (In the *Excel* vernacular, the block of cells is "named" KC.) A box in Figure 5-15 shows the range "KC."
description of value: Casing correction for the gamma-ray energy 661.66 keV and the first casing thickness (0.5625 in.).

Cell K2

program code: `=VLOOKUP(I$1,KC,5)`
action: Copies to cell K2 the value in column 5 of the row that contains \$I\$1 (=661.66) in the range "KC."
description of value: Casing correction for the gamma-ray energy 661.66 keV and the second casing thickness (0.3125 in.).

Cell K3

program code: `=VLOOKUP(I$1,KC,7)`
action: Copies to cell K3 the value in column 7 of the row that contains \$I\$1 (=661.66) in the range "KC."
description of value: Casing correction for the gamma-ray energy 661.66 keV and the third casing thickness (0.00 in.).

Cells L2, L3, N2, and P2 also have programs that retrieve values from other worksheets in this spreadsheet file.

Cell L2

program code: `=Water!C11`
action: Copies the entry in cell C11 of the "Water" worksheet to cell L2.
description of value: Depth to water, in feet.

Cell L3

program code: `=VLOOKUP(I1,KW,2)`
action: Copies to cell L3 the value in column 2 of the row that contains I1 (=661.66) in the range "KW," which is defined as *=Water*!\$B\$19:\$C\$38 (i.e., the rectangular block of cells in the "Water" worksheet with cells B19 and C38 at the corners). See Figure 8-12.
description of value: Water correction for the gamma-ray energy 661.66 keV and the water-filled 8-in.-diameter borehole.

Cell N2

program code:
action:

=VLOOKUP(I1,IE,5,0)
Copies to cell N2 the value in column 5 of the row that contains I1 (=661.66) in the range "IE," which is defined as "(E)!\$B\$17:\$F\$36. The last VLOOKUP argument, 0, indicates that the energy in the range must exactly match the value in cell I1.

description of value:

K_a value (see the Concentration Equation in Figure 8-2) for the 661.66-keV gamma ray.

Cell P2

program code:
action:

=summary!B11
Copies to cell P2 the value in cell B11 in the "Summary" worksheet.
description of value: Correction, or adjustment, for the depth.

For the worksheet illustrated in Figure 8-14, concentration calculations occur in the rows below row 4; each row corresponds to the depth indicated in column A. For example, row 5 corresponds to the depth of 238.0 ft. In row 5, cell C5 has the intensity, in counts per second, for the spectral peak associated with the 661.66-keV gamma ray. Cells J5, K5, L5, and M5 show the corrections for dead time, casing, water, and shield, respectively.

The program for cell J5 appears in the Formula Bar in Figure 8-16:

=IF(B5<10.5,1,1/(DTC!\$B\$7+DTC!\$B\$8*B5*LN(B5)+DTC!\$B\$9*B5^3)).

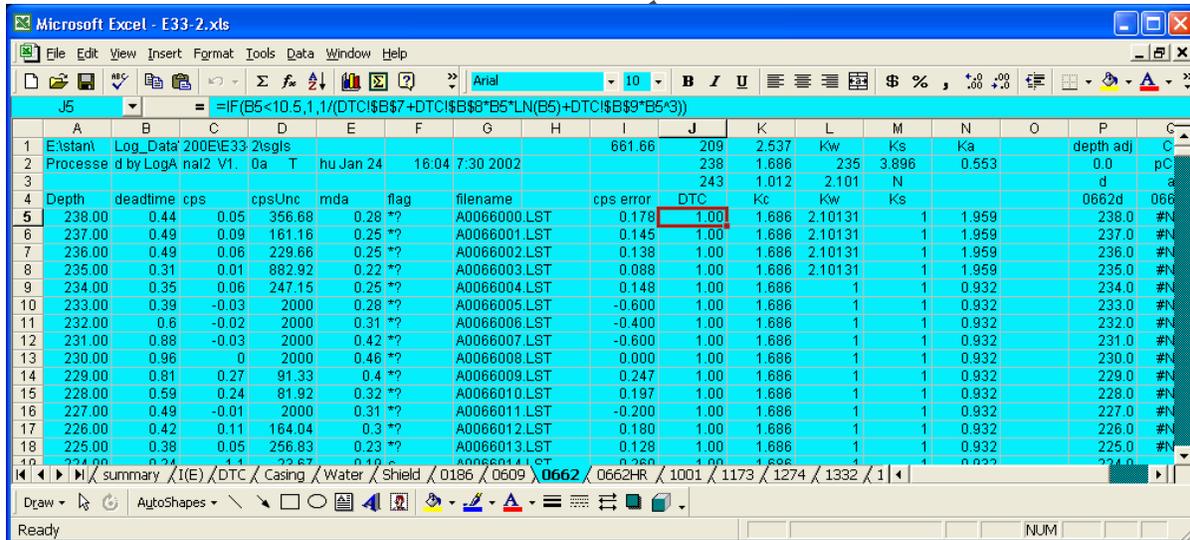


Figure 8-16. Example of Dead Time Correction for a Low Dead Time

According to this formula, the entry in cell J5 is equal to one if the value in cell B5 is less than 10.5. In this case, the value in cell B5 is 0.44, which is less than 10.5, and a value 1.00 appears in cell J5.

A dead time higher than 10.5 occurred at the depth of 51.01 ft, as indicated in cell A176 in Figure 8-17. (Figure 8-17 shows a portion of the same worksheet as pictured in Figure 8-14.)

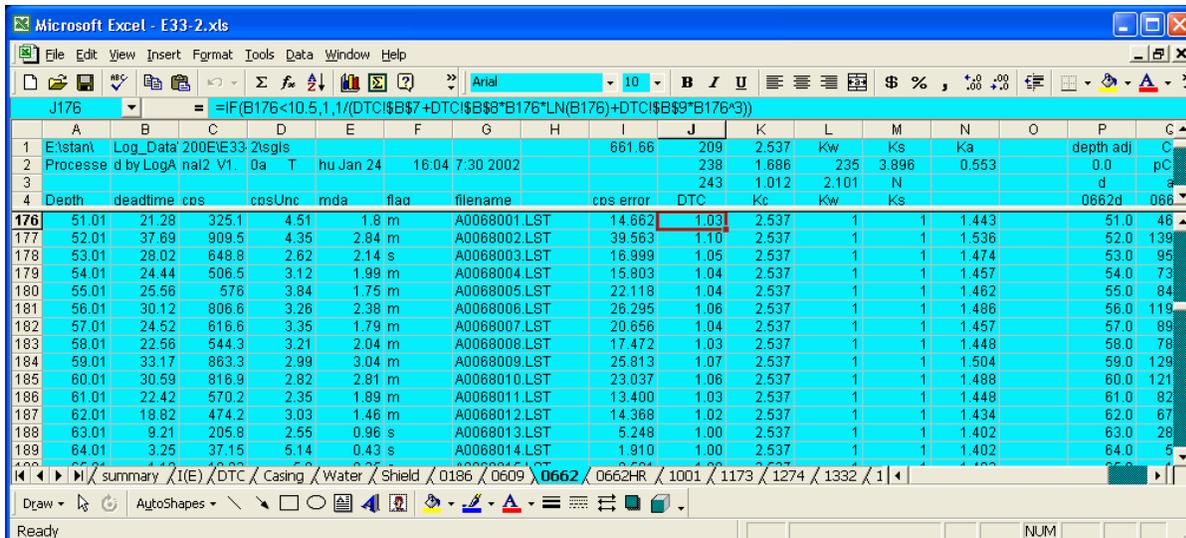


Figure 8-17. Example of Dead Time Correction for a Moderate Dead Time

For this higher dead time, the correction is greater than 1.0, and the correction is calculated as follows.

$$\begin{aligned}
 & 1/(DTC!B7+DTC!B8*B176*LN(B176) + DTC!B9*B176^3 = \\
 & 1/(DTC!B7 + DTC!B8 \times B176 \times \ln(B176) + DTC!B9 \times B176^3 = \\
 & 1/(1.008 - 4.71 \times 10^{-4} \times 21.28 \times \ln(21.28) - 5.73 \times 10^{-7} \times 21.28^3 = \\
 & 1/(1.008 - 0.010023 \times 3.05777 - 5.73 \times 10^{-7} \times 9636.401 = \\
 & 1/(1.008 - 0.030648 - 0.0055217) = 1/(0.97183) = \\
 & 1.029 \approx 1.03 = \text{the dead time correction in cell J176}
 \end{aligned}$$

Cells K1, K2, and K3 contain the corrections for the casing thicknesses 0.5625 in., 0.3125 in., and zero (no casing). The code in cells K5, K6, and below selects the proper correction, depending on the depth.

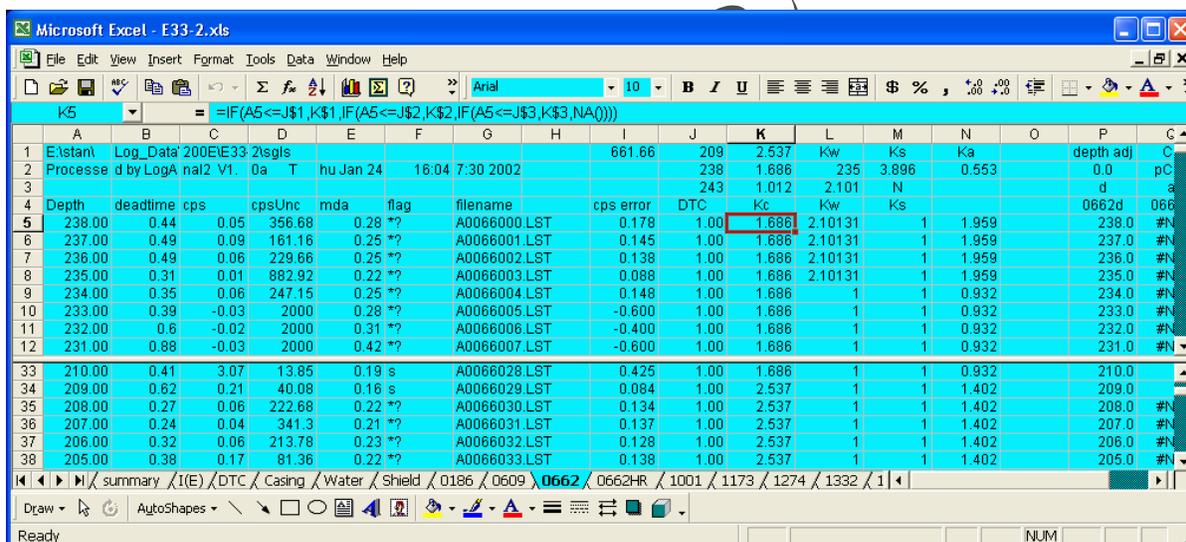


Figure 8-18. Example of Casing Correction

The Formula Bar in Figure 8-18 shows that the program for cell K5 is

`=IF(A5<=J$1, K$1,IF(A5<=J$2,K$2,IF(A5<=J$3,K$3,NA()))).`

This program copies the casing correction for the appropriate casing thickness into cell K5. The depth (cell B5) is 238.0 ft.

In Figure 8-19 the Formula Bar for the highlighted cell L5 shows the code for the water correction calculation:

`IF(ISNA(L$2),1,IF(A5<L$2,1,L$3)).`

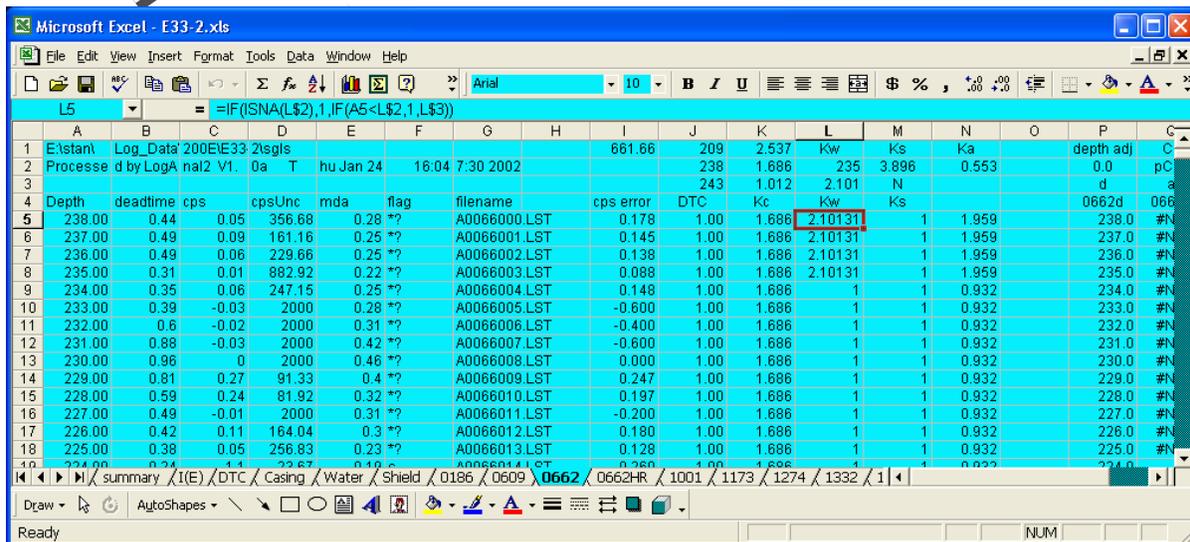


Figure 8-19. Example of Water Correction

The entry in cell L2 is the depth to water; therefore, the water correction is applicable only to data from depths greater than that shown in cell L2. Within the *IF* statement in the cell L5 code, *ISNA(L\$2)* is true if the entry in cell L2 is *N/A* (not available), i.e., if no depth to water is entered. Thus, the *IF* statement enters a value of 1 (meaning no water correction) in cell L5 if there is no water in the borehole.

If the entry in cell L2 is not *N/A*, as is the case in this example, the value in cell L5 is

`IF(A5<L$2,1,L$3).`

This value is equal to 1 if the entry in cell A5 (the depth) is less than the entry in cell L2, that is, the water correction is equal to 1 (which is no water correction) if the depth is less than the depth to water. If the depth entry in cell A5 is greater than the depth to water in cell L2, then the correction in cell L5 is the entry in cell L3. As indicated previously, cell L3 has the water correction for the gamma-ray energy 661.66 keV and the water-filled 8-in.-diameter borehole.

Equations 8-1 and 8-8 indicate that the concentration is the product of K_a and all of the corrections. The K_a value appears in the highlighted cell N2 in Figure 8-20. The Formula Bar

indicates that the K_a value was retrieved from column 5 and the row containing “661.66” (the entry in cell I1) in the block of cells named IE. The block IE is the rectangular array of cells in the IE worksheet with cells B17 and F36 at the corners (Figure 8-2).

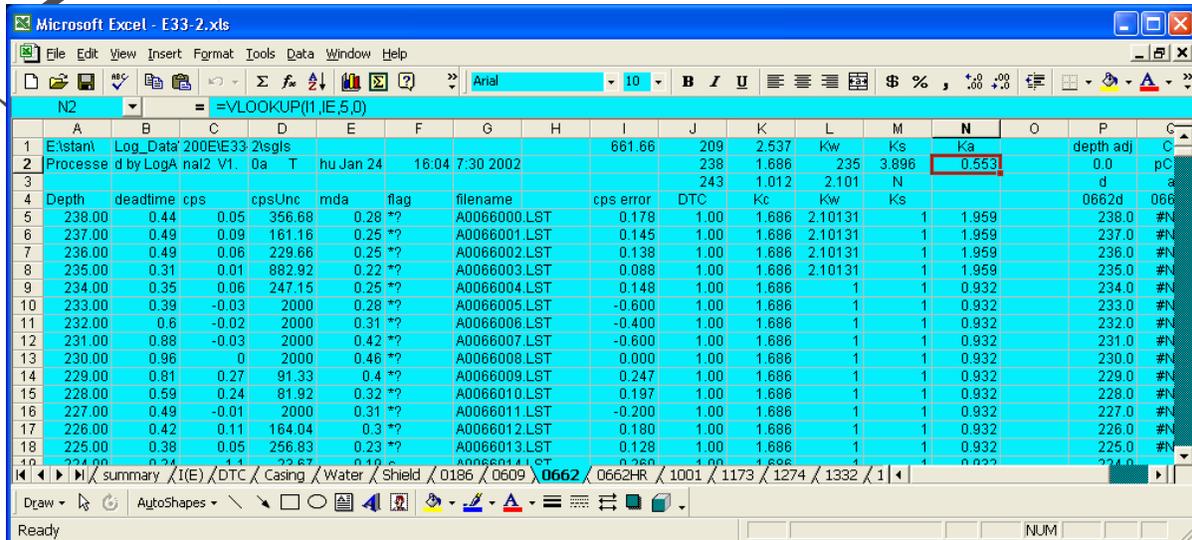


Figure 8-20. Sample K_a Value (see concentration equation in Figure 8-1)

The products of K_a and the corrections appear in cells N5, N6, N7, The Formula Bar for the highlighted cell N5 in Figure 8-23 indicates that the value in cell N5 is the product of the dead time correction (cell J5), the casing correction (cell K5), the water correction (cell L5), the shield correction (cell M5), and the K_a (cell N2). The value in cell N5 is easily verified:

$$\begin{aligned}
 &= J5 * K5 * L5 * M5 * N\$2 \\
 &= J5 \times K5 \times L5 \times M5 \times N2 = 1.00 \times 1.686 \times 2.10131 \times 0.553 \\
 &= 1.959 = \text{the value in cell N5.}
 \end{aligned}$$

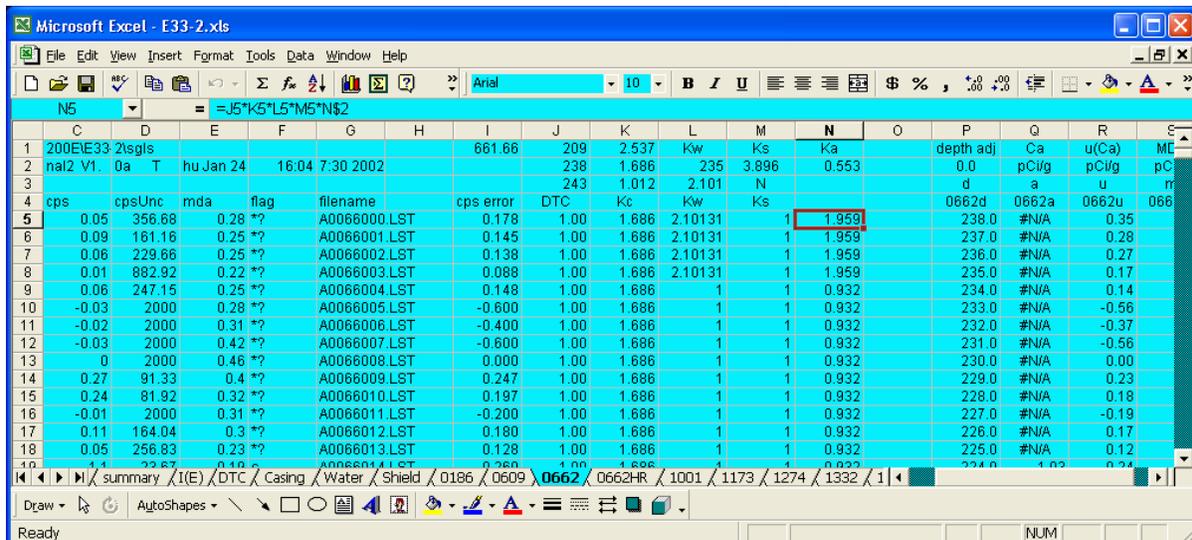


Figure 8-21. Intermediate Quantity Used in the Concentration Calculation

For the final step in the concentration calculation, calculations in row 19 instead of row 5 will be used because the peak intensity in cell C5 is less than the minimum detectable activity in cell E5.

In row 19, Figure 8-22, the concentration in cell Q19 is the product of the value in cell N19 and the peak intensity value in cell C19. The Formula Bar for Q19 indicates that the value is the product of the entries in cells N19 and C19, if the peak intensity in cell C19 is greater than the minimum detectable activity in cell E19. The verification of the concentration calculation is

$$\begin{aligned}
 &=IF(C19>E19,NA(),N19*C19) \\
 &= N19 \times C19 \text{ if } C19 > E19, \text{ or } NA \text{ if } C19 < E19 \\
 &= N19 \times C19 \text{ because } C19 > E19 \\
 &= 0.932 \times 1.1 = 1.025 \approx 1.03 = \text{the value in Q19.}
 \end{aligned}$$

In row 18, the peak intensity in cell C18 is less than the minimum detectable activity in cell E18, so the concentration has not been calculated and the entry #N/A appears in cell Q18.

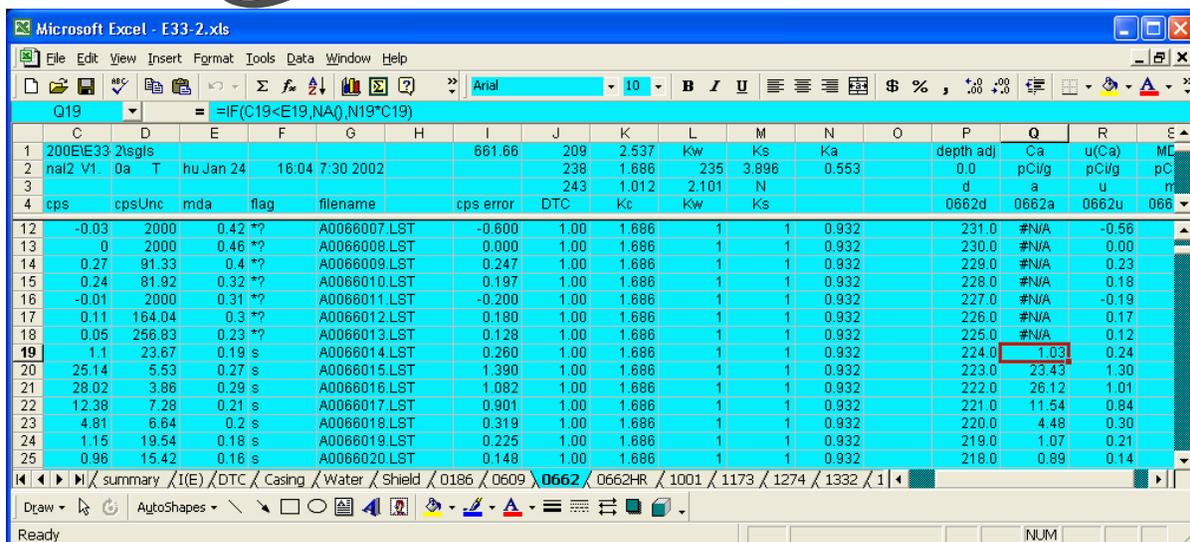


Figure 8-22. Example of Calculated ¹³⁷Cs Concentration

8.4.6.2 Concentration Uncertainties

As stated in Section 8.3.3, systematic uncertainties are not included in the concentration uncertainty calculations. The concentration uncertainties are based on the statistical uncertainties in recorded spectral peak counts. The expression for the concentration uncertainty is

$$\sigma C_a = C_a \times \sqrt{\left(\frac{\sigma P_n}{P_n}\right)^2} = C_a \times \frac{\sigma P_n}{P_n}$$

(Equation 8-7).

C_a is the concentration, which is calculated with Equation 8-1, and P_n and σP_n are the peak intensity and the uncertainty in the intensity, respectively. Values for P_n are calculated by

PCMCA/WIN. PCMCA/WIN also calculates an uncertainty for each P_n value; each uncertainty is expressed as a percentage of P_n . In the sample PCMCA/WIN output file in Example 1, the P_n values are in the “Activity” column and the uncertainties are in the “Error” column.

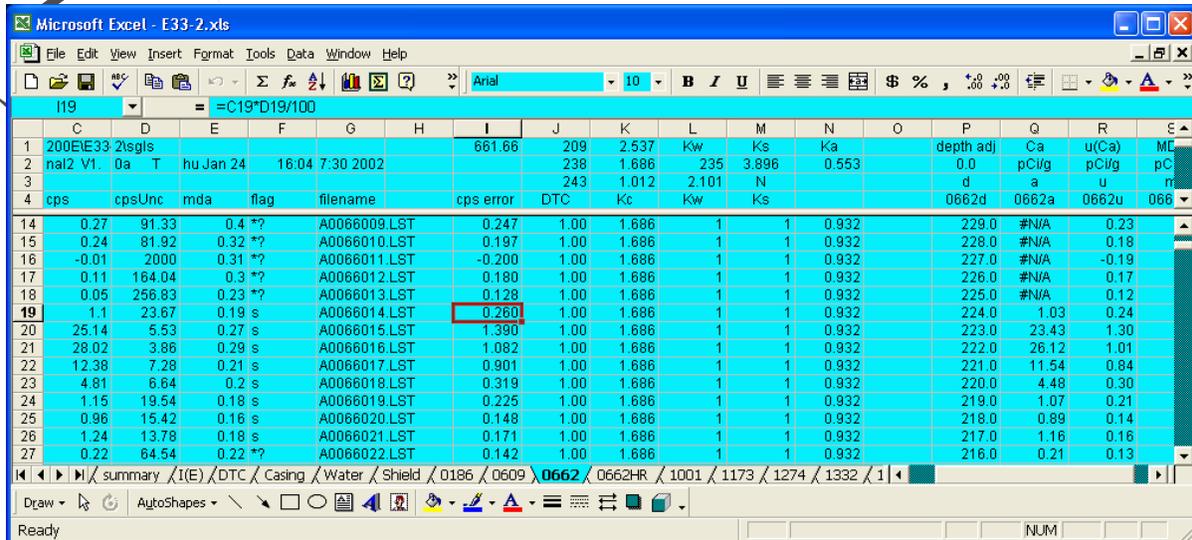


Figure 8-23. Example of Calculation of Absolute Peak Intensity Uncertainty

In Figure 8-23, the peak intensity uncertainties from PCMCA/WIN output files have been compiled in column D. The corresponding absolute uncertainties, i.e., the σP_n values, appear in column I. For the highlighted cell I19, the Formula Bar shows how the absolute uncertainty is calculated for the intensity in cell C19:

$$=C19*D19/100$$

$$= C19 \times (D19/100) = 1.1 \times (23.67/100) = 0.260 = \text{the value in cell I19.}$$

The entry in cell I19 is the σP_n value, in counts per second, associated with the peak intensity in cell C19.

The highlighted cell R19 in Figure 8-24 has the concentration uncertainty associated with the concentration in cell Q19. The Formula Bar indicates that the value is the product of the values in cells N19 and I19, which is easily verified:

$$=N19*I19$$

$$= N19 \times I19 = 0.932 \times 0.260 = 0.242 \approx 0.24 = \text{the value in cell R19}$$

Figure 8-24. Example of Calculation of ^{137}Cs Concentration Uncertainty

That $N19 \times I19$ is equal to σC_a (Equation 8-7) is demonstrated as follows. $N19 \times I19$ is equal to

$$J19 \times K19 \times L19 \times M19 \times N2 \times I19,$$

which is

$$N19 \times I19 = K_{DT} \times K_C \times K_W \times K_S \times \frac{27.027}{Y} \times I(E) \times \sigma P_n.$$

Also,

$$K_{DT} \times K_C \times K_W \times K_S \times \frac{27.027}{Y} \times I(E) \times P_n = C_a.$$

Therefore,

$$N19 \times I19 = C_a \times \frac{\sigma P_n}{P_n} = \sigma C_a.$$

8.4.7 Minimum Detectable Level

Section 8.3.4 described the MDL (minimum detectable level) as the radionuclide concentration associated with the smallest spectral peak for which detection is statistically defensible. Concentrations are normally derived from peak intensities, using calculations outlined in Section 8.3.2, but in the case of MDLs, *PCMCA/WIN* does not identify peaks or calculate peak intensities. Instead of peak intensities, the calculations employ MDA (minimum detectable activity) values, which are essentially the intensities of the smallest spectral anomalies that can

be identified as peaks by *PCMCA/WIN*. These anomalies do not actually exist in the spectra. For each particular spectral region of interest (ROI), *PCMCA/WIN* estimates the size of the smallest anomaly that would stand high enough above background to be identified as a peak. Each estimation is based on statistical analyses of several parameters, the most important of which is the character of the background counts over the ROI.

Two MDA analyses are normally performed in routine spectrum analysis. These analyses use different methods to establish ROIs. For the “Activities with MDA” analysis, spectral peaks are identified by the *Peaksearch* algorithm, then ROIs are set so that each peak is spanned by an ROI. Within each ROI, the peak itself is ignored and the background and other parameters are used to calculate an MDA value in counts per second.

The second analysis, which is called “Allow Identification to create ‘Force MDA’ ROIs with an ROI width of 2.07892 times Γ 's (sic) FWHM,” establishes ROIs for gamma rays that are listed in the source identification library file but are not represented by peaks in a spectrum. The spectra must be energy calibrated and resolution calibrated before analysis begins. *PCMCA/WIN* determines positions of ROI centers by reading the gamma-ray energies in the library file, then using those energies and the spectrum energy calibration to determine the MCA channel numbers that correspond to the energies. The width of each ROI is 2.07892 times a full width at half maximum (FWHM) value that is calculated using the spectrum resolution calibration and the number of the MCA channel at the center of the ROI. After the position and width of each ROI is set, *PCMCA/WIN* uses the background and other parameters to calculate an MDA value in counts per second for each ROI. The ROI width of 2.07892 times full width at half maximum is customarily used, though the value can be changed by the analyst.

Figure 8-25 shows a worksheet in which column E lists MDAs that have been calculated by *PCMCA/WIN* for the 661.6-keV gamma ray of ^{137}Cs .

Depth	deadtime	cps	cpsUnc	mda	flag	filename	cps error	DTC	Kc	Kw	Ks	depth adj	0662d	066
161	179	0.38	0.18	82.75	0.24	??	A0067084.LST	0.149	1.00	2.537	1	1.402	179.0	#N
162	180	0.45	0.14	104.95	0.24	??	A0067085.LST	0.147	1.00	2.537	1	1.402	180.0	#N
163	181	0.32	0.07	204.69	0.25	??	A0067086.LST	0.143	1.00	2.537	1	1.402	181.0	#N
164	182	0.42	0.06	226.62	0.24	??	A0067087.LST	0.136	1.00	2.537	1	1.402	182.0	#N
165	183	0.38	0.04	365.08	0.26	??	A0067088.LST	0.146	1.00	2.537	1	1.402	183.0	#N
166	184	0.41	0	2000	0.24	??	A0067089.LST	0.000	1.00	2.537	1	1.402	184.0	#N
167	185	0.3	0.08	182.91	0.24	??	A0067090.LST	0.146	1.00	2.537	1	1.402	185.0	#N
168	186	0.37	0.02	572.61	0.24	??	A0067091.LST	0.115	1.00	2.537	1	1.402	186.0	#N
169	187	0.7	0.02	818.64	0.24	??	A0067092.LST	0.164	1.00	2.537	1	1.402	187.0	#N
170	188	0.42	0.15	93.74	0.22	??	A0067093.LST	0.141	1.00	2.537	1	1.402	188.0	#N
171	189	0.28	0.08	173.05	0.23	??	A0067094.LST	0.138	1.00	2.537	1	1.402	189.0	#N
172	190	0.3	0.06	241.4	0.23	??	A0067095.LST	0.145	1.00	2.537	1	1.402	190.0	#N
173	191	0.38	0.05	286.69	0.24	??	A0067096.LST	0.143	1.00	2.537	1	1.402	191.0	#N
174	192	0.37	0.12	112.33	0.23	??	A0067097.LST	0.135	1.00	2.537	1	1.402	192.0	#N
175	50.01	3.49	21.16	8.52	0.41	s	A0068000.LST	1.803	1.00	2.537	1	1.402	50.0	2
176	51.01	21.28	325.1	4.51	1.8	m	A0068001.LST	14.662	1.03	2.537	1	1.443	51.0	46
177	52.01	37.69	909.5	4.35	2.84	m	A0068002.LST	39.563	1.10	2.537	1	1.536	52.0	139
178	53.01	28.02	648.8	2.62	2.14	s	A0068003.LST	16.999	1.05	2.537	1	1.474	53.0	95
179	54.01	24.44	506.5	3.12	1.99	m	A0068004.LST	15.803	1.04	2.537	1	1.457	54.0	73
180	55.01	25.56	576	3.84	1.75	m	A0068005.LST	22.118	1.04	2.537	1	1.462	55.0	84

Figure 8-25. MDA Examples

The highlighted cell C166 of the worksheet depicted in Figure 8-25 shows a zero entry for the peak intensity. The corresponding spectrum did not have a discernible peak for the 661.6-keV ^{137}Cs gamma ray, but the source identification library file had an entry for the gamma ray. Thus, *PCMCA/WIN* set an ROI at the position where the peak would exist and determined the MDA of 0.24 in cell E166. The background across the ROI was relatively smooth so the MDA is relatively small.

The cell C177 shows a large value (909.5) for the 661.6-keV gamma-ray peak intensity. This peak was identified by *Peaksearch*, then *PCMCA/WIN* used the ROI surrounding the peak to calculate the MDA. The presence of the peak made the background more difficult to determine, so the MDA in cell E177 is relatively large.

Figure 8-26 shows a different part of the same worksheet displayed in Figure 8-25. Column S displays the calculated MDL values.

	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	2tsjls						661.66	209	2.537	Kw	Ks	Ka		depth adj	Ca	u(Ca)	MDL
2	0a T	hu Jan 24	16.04	7:30 2002				238	1.686	235	3.896	0.553	d	pCi/g	a	pCi/g	pCi/g
3								243	1.012	2.101	N		0662d	0662a	0662u	0662m	
4	cpsUnc	mda	flag	filename		cps error	DTC	Kc	Kw	Ks			0662d	0662a	0662u	0662m	
161	82.75	0.24	**	A0067084.LST		0.149	1.00	2.537	1	1	1.402		179.0	#N/A	0.21	0.34	
162	104.85	0.24	**	A0067085.LST		0.147	1.00	2.537	1	1	1.402		180.0	#N/A	0.21	0.34	
163	204.69	0.25	**	A0067086.LST		0.143	1.00	2.537	1	1	1.402		181.0	#N/A	0.20	0.35	
164	226.62	0.24	**	A0067087.LST		0.136	1.00	2.537	1	1	1.402		182.0	#N/A	0.19	0.34	
165	365.08	0.26	**	A0067088.LST		0.146	1.00	2.537	1	1	1.402		183.0	#N/A	0.20	0.36	
166	2000	0.24	**	A0067089.LST		0.000	1.00	2.537	1	1	1.402		184.0	#N/A	0.00	0.34	
167	182.91	0.24	**	A0067090.LST		0.146	1.00	2.537	1	1	1.402		185.0	#N/A	0.21	0.34	
168	572.61	0.24	**	A0067091.LST		0.115	1.00	2.537	1	1	1.402		186.0	#N/A	0.16	0.34	
169	818.64	0.24	**	A0067092.LST		0.164	1.00	2.537	1	1	1.402		187.0	#N/A	0.23	0.34	
170	93.74	0.22	**	A0067093.LST		0.141	1.00	2.537	1	1	1.402		188.0	#N/A	0.20	0.31	
171	173.05	0.23	**	A0067094.LST		0.138	1.00	2.537	1	1	1.402		189.0	#N/A	0.19	0.32	
172	241.4	0.23	**	A0067095.LST		0.145	1.00	2.537	1	1	1.402		190.0	#N/A	0.20	0.32	
173	286.69	0.24	**	A0067096.LST		0.143	1.00	2.537	1	1	1.402		191.0	#N/A	0.20	0.34	
174	112.33	0.23	**	A0067097.LST		0.135	1.00	2.537	1	1	1.402		192.0	#N/A	0.19	0.32	
175	8.52	0.41	s	A0068000.LST		1.803	1.00	2.537	1	1	1.402		50.0	29.68	2.53	0.58	
176	4.51	1.0	m	A0068001.LST		14.662	1.03	2.537	1	1	1.443		51.0	469.16	21.16	2.60	
177	4.35	2.84	m	A0068002.LST		39.563	1.10	2.537	1	1	1.536		52.0	1397.25	60.78	4.36	
178	2.62	2.14	s	A0068003.LST		16.999	1.05	2.537	1	1	1.474		53.0	956.39	25.06	3.15	
179	3.12	1.99	m	A0068004.LST		15.803	1.04	2.537	1	1	1.457		54.0	737.76	23.02	2.90	
180	3.84	1.75	m	A0068005.LST		22.118	1.04	2.537	1	1	1.462		55.0	841.99	32.33	2.56	

Figure 8-26. Examples of MDL Values

The highlighted cell S166 shows the MDL value derived from the MDA value in cell E166. The MDAs and other quantities calculated by *PCMCA/WIN* do not require verification, but the MDL calculation is programmed in the spreadsheet and does require verification. The formula bar indicates that the MDL value in cell S166 is the product of the MDA value in cell E166 and the K_a value in cell N166. This calculation is equivalent to the concentration calculation described in Sections 8.3.2 and 8.4.1, except the K_a value is multiplied by the MDA instead of a spectral peak intensity. The entry in cell S166 is easily verified:

$$=N166 * E166$$

$$= N166 \times E166 = 1.402 \times 0.24 = 0.336 \approx 0.34 = \text{the value in cell S166.}$$

This concludes the verification of calculations programmed in the 0662 worksheet. Calculations in the other concentration worksheets (186, 609, 0662HR, 1001, 1173, 1274, 1332, 1408, 1461, 1764, and 2615) need not be separately verified because those worksheets are “clones” of the 0662 worksheet. That is, the calculation programmed in any cell of any concentration worksheet is identical to the calculation programmed in the analogous cell of the 0662 concentration worksheet.

In Figure 8-27, the “tabs” in a line near the bottom of the worksheet show that there are additional worksheets named *grosscnt*, *grosscnt (HR)*, *GG&DT*, *MM*, *KUT*, *Kc Plot*, and *log*. These worksheets have data summaries, compilations of data, and graphs. There are no calculations that require verification. For example, the *GG&DT* (gross gamma and dead time) worksheet illustrated in Figure 8-27 has graphs that show gross gamma-ray count rates and dead time values plotted in relation to depth.

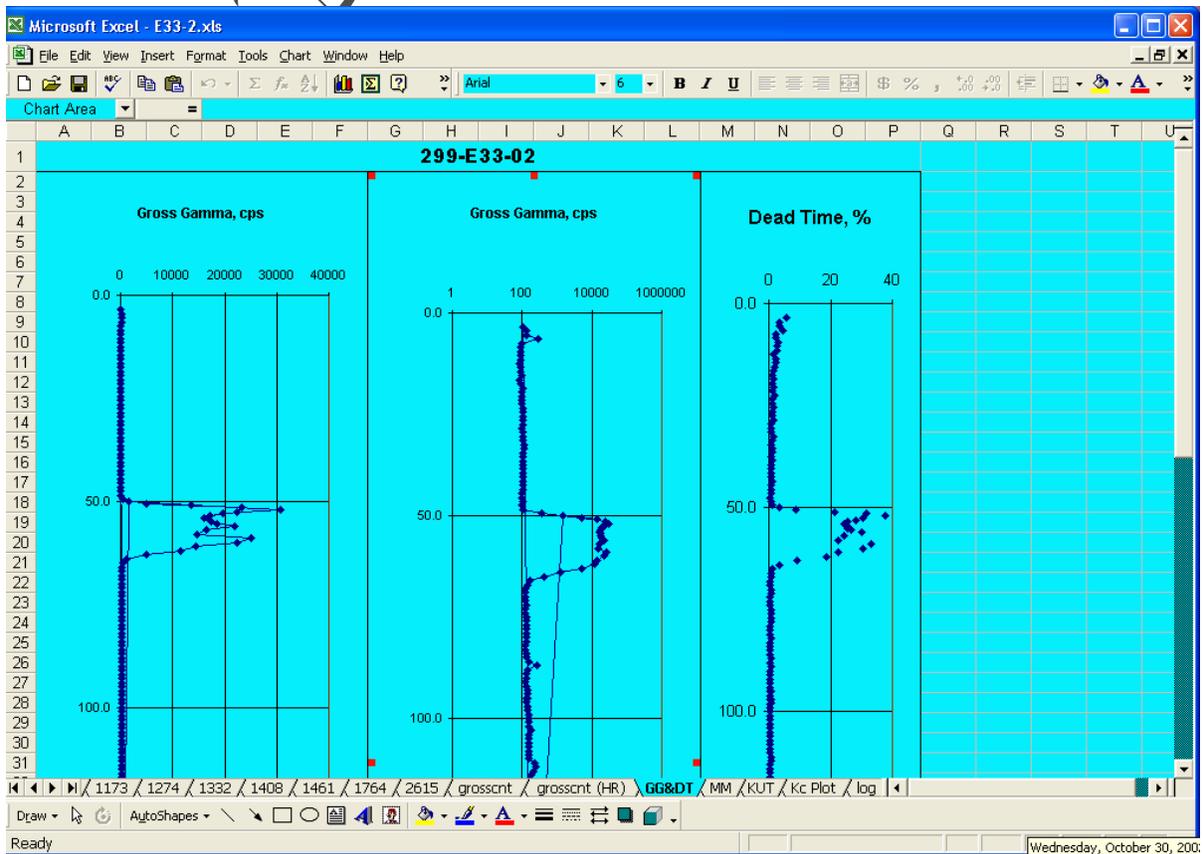


Figure 8-27. Part of the GG&DT (Gross Gamma and Dead Time) Worksheet

9.0 Version Control and Revision History

The versions of software used in data analysis (i.e., *Aptec*, *Excel*) are controlled and recorded for quality purposes. This ensures that only approved software is used for data analysis and that the version of a program can be recalled. The project system administrator is responsible for providing approved versions of software for data analysis.

The project will attempt to maintain the most current version of commercial software. Use of the most current version offers many benefits, the most important being the ability to obtain support from vendors when necessary. For in-house software, all analysis will be performed with the most current version. Old versions of software should not be used to process data.

The following sections list specific versions of software that are being used by the project at the time of manual revision. Project-specific software is noted as applicable.

9.1 Commercial Application Software

9.1.1 Access 2000

Access (Microsoft) is a database program used to facilitate selection and prioritization of borehole monitoring intervals for the Hanford Tank Farms Vadose Zone Monitoring Project.

9.1.2 Excel 2000

Excel 2000 (Microsoft) is a spreadsheet program used for the Hanford 200 Areas Spectral Gamma Vadose Zone Characterization Project to convert radionuclide count rates measured by the SGLS to radionuclide concentrations. Calibration factors and dead-time and environmental corrections are applied to the count-rate data to calculate radionuclide concentrations assumed to be evenly distributed in the earth around the borehole. *Excel* is also used to track SGLS field verification information.

The Hanford Tank Farms Vadose Zone Monitoring Project uses *Excel* to plot data generated by the Radionuclide Assessment System (RAS) software. *Excel* is also used to apply corrections for radioactive decay and to compare data from successive log runs.

9.1.3 Word 2000

Word 2000 (Microsoft) is a program used for word processing.

9.1.4 Adobe Acrobat

Adobe Acrobat, Version 5.0, (Adobe Systems, Inc.) is a program used to generate a portable document format (*.pdf) file that can be sent via email or downloaded from the project web site.

9.1.5 *SigmaPlot*

SigmaPlot 8.0 (SPSS, Inc.) is the plotting software used by the Hanford 200 Areas Spectral Gamma Vadose Zone Characterization Project to generate plots of radionuclide concentrations.

9.1.6 *Aptec*

Aptec, Version 6.31, Release 14 (Canberra Co.), is used by the Hanford 200 Areas Spectral Gamma Vadose Zone Characterization Project to convert data recorded by the SGLS as *.CHN to *.LST files from which the *rdaptec* program can extract analysis results that are imported into *Excel* for further data analysis.

9.1.7 *Environmental Visualization System (EVS)*

EVS, Version 5.51, (C Tech Development Corporation), is the modeling software used by the Hanford 200 Areas Spectral Gamma Vadose Zone Characterization Project to create three-dimensional visualizations.

9.2 Operating System Software

9.2.1 Server

The computer workstations are on a network with a dedicated server running *Windows 2000* (Microsoft).

9.2.2 Workstation

All analysts' workstations use *Windows 2000* (Microsoft).

9.3 In-House Software

9.3.1 *SGLSoffline*

SGLSoffline, Version 1.0a, is a program developed to assemble a set of SGLS spectra that exist as individual files for each depth increment into a set of log type files, one for each isotope found during spectrum analysis.

UNCLASSIFIED

**Appendix A
Radionuclide Data**

Radionuclide Data

Gamma energy levels and gamma yields associated with radioactive decay are required for identification and quantification of naturally occurring and man-made radionuclides. Gamma energy and yield values are obtained from Firestone and Shirley (1996), which is available for staff use in both hard copy and CD-ROM versions. Updated values of radionuclide parameters are available from the Internet, but published values from Firestone and Shirley (1996) will be used to promote consistency and traceability in log data. Tables A-1 and A-2 provide lists of significant gamma lines of interest. More detailed tables are provided for use by the analysts, sorted by either radionuclide or gamma energy value. For gamma energy values expressed in kilo-electron-volts (keV), two decimal places is sufficient accuracy. Note that gamma yield values are frequently expressed in percent (gammas per 100 decays). However, the quantity γ used in the concentration equation is expressed in gammas per decay; this is always a number between 0 and 1.

Within *Aptec PC/MCA/Win*, the *Identify Peaks* routine uses information stored in a library file (*.LIB) to identify each peak by matching the closest energy line. *Identify Peaks* is generally set up to run with a tolerance of $\approx 3-4$ keV, and peaks may be misidentified if energy levels are too close together. For this reason, library files have been edited to remove selected peaks where the difference in gamma energy level is less than about 5 keV. Three *Aptec* library files are available for use in spectral analysis: KUT.LIB, SGLS.LIB, and HRLS.LIB. Both KUT.LIB and SGLS.LIB are used with the SGLS. The KUT.LIB file lists naturally occurring radionuclides and primarily is used for processing of verification spectra. In cases of two closely spaced peaks, preference is given to peaks associated with naturally occurring radionuclides. SGLS.LIB is used for processing of SGLS log spectra. In cases of two closely spaced peaks, preference is given to peaks associated with man-made radionuclides, unless the natural gamma line is relatively prominent. HRLS.LIB is used for processing both HRLS verification and log spectra. It contains an abbreviated list of radionuclides, with preference given to peaks associated with man-made radionuclides. The last three columns in Tables A-1 and A-2 indicate which gamma lines are included in each of the three libraries. An "MDA" in the library column indicates that a region of interest is "forced" for that gamma line, and an MDA will be computed, even if no peak is detected when "Create force MDA" is checked under peak identification parameters. Note that half life and yield values in these library files do not correspond exactly with values from Firestone and Shirley (1996). This is due to the way data values are stored in the *Aptec* library files. Note also that the "convert factor" is set at 0 for all radionuclides. This has no effect, because radionuclide concentration values are calculated independently of the *Aptec* software. Values for half-life, yield, and "convert factor" stored in the library file are not used in calculations and can be ignored.

Gamma energy levels are the primary diagnostic factor in identification of unknown radionuclides, and nuclear data may be required for other purposes. Given below are annotated sources of radionuclide data on the Internet (as of April 2002).

The Isotopes Project -- <http://ie.lbl.gov/>. The Isotopes Project compiles, evaluates, and disseminates nuclear structure and radioactive decay data for basic and applied research.

Lund/LBNL Table of Isotopes -- <http://ie.lbl.gov/toi.html>. A good starting point for nuclear data. Links to a wide variety of data sources. The handbook *Table of Isotopes* has for many years been the most widely used source of information for nuclear structure and decay data. Please refer to this link for information about the book, the CD-ROM, and also additional tables and information on nuclear data. This service is intended to give convenient Web access to the *Table of Isotopes* data. At present only part of the decay data are implemented, but the service will eventually include search facilities, table generators, charts and drawings of all nuclear structure and decay data in the *Table of Isotopes* book.

The Lund/LBNL Nuclear Data Search -- <http://nucleardata.nuclear.lu.se/NuclearData/toi/>. Provides the capability to search by alpha or gamma energy level.

National Nuclear Data Center -- <http://www.nndc.bnl.gov/>. The National Nuclear Data Center (NNDC) is funded by the U.S. Department of Energy to provide information services in the fields of low- and medium-energy nuclear physics to users in the United States and Canada. In particular, the Center can provide information on neutron, charged-particle, and photonuclear reactions, nuclear structure, and decay data.

U.S. Nuclear Data Program -- <http://www.nndc.bnl.gov/usndp/>. The U.S. Nuclear Data Program (USNDP), a DOE-funded project, brings together a number of Laboratories to assemble, maintain, and disseminate a unified body of nuclear data to be used to support basic nuclear research and a wide variety of nuclear applications. These data include nuclear structure and nuclear reaction data, the decay properties of nuclei, nuclear masses, and astrophysical reaction rates.

Gamma Spectrometry Center -- <http://id.inel.gov/gamma/>. This site includes integrated technical reference material of gamma energies, decay spectra, and actual spectra in catalog form, history of gamma-ray spectrometry at the INEEL, and links to other sources of nuclear data.

Radiation Information Network -- <http://www.physics.isu.edu/radinf/>. Emphasis on radiation protection information. Links to a wide range of sites.

RSO Toolbox -- <http://www.physics.isu.edu/radinf/rsotoolbox.htm>

RadWaste.org -- <http://www.radwaste.org/index.html>

NIST Physical Reference Data -- <http://physics.nist.gov/PhysRefData/contents.html>

Canberra -- <http://www.canberra.com/index2.htm>. Canberra is a major supplier of analytical instruments, systems, and services for radiation measurement. Applications for Canberra offerings include health physics, nuclear power operations, Radiation Monitoring Systems (RMS), nuclear safeguards, nuclear waste management, environmental radiochemistry and other areas. As a part of the recently formed, \$9 Billion Areva group, the new Canberra has been formed from three previous companies - Canberra Industries, Aptec-NRC, and Eurisys Mesures.

The site includes technical articles and guidance on various aspects of radiation detection and measurement.

Ortec -- <http://www.ortec-online.com/>. ORTEC is a provider of detectors, pulse-processing electronics, software, and spectrometers for measuring and quantifying the energy and time distributions of optical photons, X rays, gamma rays, charged particles, and radioactive nuclides...in the laboratory or the natural environment.

Detector Portal -- <http://www.detectorportal.net/>. Detectorportal.net is a unique service established to provide a focused resource combining the information on light and radiation detectors and their use, technical application notes, selection charts, and detector sourcing resources with online quote and purchasing capability.

Table A-1. Radionuclide Data Sorted by Nuclide and Yield

Name	Energy	Desc	Yield (%)	Half Life	KUT	SGLS	HRLS
K-40	1460.83		10.67	1.28E+09 yrs	MDA	MDA	x
Th-232	288.63	Pb-212	43.3	1.41E+10 yrs	MDA	x	x
Th-232	2614.53	Tl-208	35.34	1.41E+10 yrs	MDA	MDA	
Th-232	583.19	Tl-208	30.11	1.41E+10 yrs	MDA	MDA	x
Th-232	911.21	Ac-228	26.6	1.41E+10 yrs	MDA	x	
Th-232	968.97	Ac-228	16.17	1.41E+10 yrs	MDA	x	
Th-232	338.32	Ac-228	11.25	1.41E+10 yrs	MDA	x	
Th-232	510.77	Tl-208	8.06	1.41E+10 yrs	MDA		
Th-232	727.33	Bi-212	6.58	1.41E+10 yrs	x		
Th-232	964.77	Ac-228	5.11	1.41E+10 yrs	x		
Th-232	463.01	Ac-228	4.44	1.41E+10 yrs	x		
Th-232	860.56	Tl-208	4.43	1.41E+10 yrs	x		
Th-232	794.95	Ac-228	4.34	1.41E+10 yrs	x		
Th-232	240.99	Ra-224	3.97	1.41E+10 yrs	x		
Th-232	209.25	Ac-228	3.88	1.41E+10 yrs	x		
Th-232	270.24	Ac-228	3.43	1.41E+10 yrs	x		
Th-232	306.09	Pb-212	3.28	1.41E+10 yrs	x		
Th-232	1588.21	Ac-228	3.27	1.41E+10 yrs	x	x	
Th-232	328	Ac-228	2.95	1.41E+10 yrs	x		
Th-232	129.07	Ac-228	2.45	1.41E+10 yrs	x		
Th-232	277.36	Tl-208	2.27	1.41E+10 yrs	x		
Th-232	409.46	Ac-228	1.94	1.41E+10 yrs	x		
Th-232	835.71	Ac-228	1.65	1.41E+10 yrs	x		
Th-232	1630.63	Ac-228	1.6	1.41E+10 yrs	x	x	
Th-232	772.29	Ac-228	1.5	1.41E+10 yrs	x		
Th-232	1620.5	Bi-212	1.49	1.41E+10 yrs	x	x	
Th-232	99.5	Ac-228	1.28	1.41E+10 yrs	x		
Th-232	84.37	Ac-228	1.27	1.41E+10 yrs	x		
Th-232	785.37	Bi-212	1.1	1.41E+10 yrs	x		
Th-232	755.32	Ac-228	1.01	1.41E+10 yrs	x		
Th-232	726.86	Ac-228	0.64	1.41E+10 yrs	x		
U-238	609.31	Bi-214	44.79	4.47E+09 yrs	MDA	MDA	x
U-238	351.92	Pb-214	35.8	4.47E+09 yrs	MDA	x	x
U-238	295.21	Pb-214	18.5	4.47E+09 yrs	MDA	x	
U-238	1764.49	Bi-214	15.36	4.47E+09 yrs	MDA	MDA	
U-238	1120.29	Bi-214	14.8	4.47E+09 yrs	MDA	x	
U-238	241.98	Pb-214	7.5	4.47E+09 yrs	x		
U-238	1238.11	Bi-214	5.86	4.47E+09 yrs	x		
U-238	2204.21	Bi-214	4.86	4.47E+09 yrs	MDA	x	
U-238	768.36	Bi-214	4.8	4.47E+09 yrs	x		
U-238	1377.67	Bi-214	3.92	4.47E+09 yrs	x		
U-238	186.1	Ra-228	3.5	4.47E+09 yrs	MDA		
U-238	934.06	Bi-214	3.03	4.47E+09 yrs	x	x	
U-238	1729.6	Bi-214	2.88	4.47E+09 yrs	x	x	
U-238	92.38	Th-234	2.81	4.47E+09 yrs	x		
U-238	1407.98	Bi-214	2.8	4.47E+09 yrs	x		
U-238	92.8	Th-234	2.77	4.47E+09 yrs	x		
U-238	1509.23	Bi-214	2.12	4.47E+09 yrs	x	x	
U-238	1847.42	Bi-214	2.04	4.47E+09 yrs	x	x	
U-238	1155.19	Bi-214	1.64	4.47E+09 yrs	x		
U-238	1401.5	Bi-214	1.55	4.47E+09 yrs	x		
U-238	2447.86	Bi-214	1.5	4.47E+09 yrs	MDA	x	
U-238	665.45	Bi-214	1.29	4.47E+09 yrs	x		
U-238	1661.28	Bi-214	1.14	4.47E+09 yrs	x	x	
U-238	2118.55	Bi-214	1.14	4.47E+09 yrs	x	x	
U-238	806.17	Bi-214	1.12	4.47E+09 yrs	x		
U-238	785.91	Pb-214	0.85	4.47E+09 yrs	x		

Table A-1. Radionuclide Data Sorted by Nuclide and Yield

Name	Energy	Desc	Yield (%)	Half Life	KUT	SGLS	HRLS
U-238	1001	Pb-214	0.84	4.47E+09 yrs	x		
Co-60	1332.5		99.98	5.271 yrs		x	x
Co-60	1173.24		99.9	5.271 yrs		x	x
Ru-106	621.93	Rh-106	9.93	373.643 day		x	x
Sb-125	427.88		29.6	2.7582 yrs		x	x
Sb-125	600.6		17.86	2.758 yrs		x	
Sb-125	635.95		11.31	2.7582 yrs		x	
Sb-125	468.37		10.49	2.7582 yrs		x	
Sb-125	176.31		6.82	2.758 yrs		x	
Sn-126	666.1		86	100000 yrs		x	x
Sn-126	694.8		82.56	100000 yrs		x	
Cs-134	604.7		97.56	2.062 yrs		x	x
Cs-134	795.85		85.44	2.062 yrs		x	x
Cs-137	661.66		85.1	30.07 yrs	x	MDA	MDA
Eu-152	121.78		28.42	13.542 yrs		x	
Eu-152	344.28		26.58	13.54 yrs		x	x
Eu-152	1408.01		20.87	13.54 yrs		x	x
Eu-152	1112.12		13.54	13.54 yrs		x	
Eu-152	778.9		12.96	13.54 yrs		x	
Eu-154	123.07		40.79	8.593 yrs		x	
Eu-154	1274.44		35.19	8.593 yrs		x	x
Eu-154	723.31		20.22	8.593 yrs		x	x
Eu-154	873.19		12.27	8.593 yrs		x	
Eu-155	105.31		21.15	4.7611 yrs		x	
U-235	185.72		57.2	7.04E+08 yrs		x	x
U-235	143.76		10.96	7.04E+08 yrs		x	
U-235	163.33		5.08	7.04E+08 yrs		x	
U-235	205.31		5.01	7.04E+08 yrs		x	
Np-237	312.17	Pa-233	38.6	2.14E+06 yrs		x	x
Np-237	86.48		12.4	4.761 yrs		x	
Np-237	300.34	Pa-233	6.62	1.41E+10 yrs		x	
U-238p	1001.03	Pa-234	0.84	4.47E+09 yrs		x	x
U-238p	811	Pa-234	0.51	4.47E+09 yrs		x	x
U-238p	766.36	Pa-234	0.29	4.47E+09 yrs		x	x
Pu-239	51.62		0.0271	24110 yrs		x	x
Pu-239	129.3		0.0063	24110 yrs		x	x
Pu-239	375.05		0.0016	24110 yrs		x	x
Pu-239	98.78		0.0012	24110 yrs		x	
Am-241	59.54		35.9	432.2 yrs		x	x

Notes:

- i. For natural radionuclides, all lines are associated with the parent radionuclide (^{238}U or ^{232}Th) and the half-life of the parent is given. The daughter radionuclide from which the gamma is emitted is indicated in the description column.
- ii. Yields for ^{208}Tl are adjusted to account for the branching ratio (0.3594) for the decay of ^{212}Bi to ^{208}Tl . All other branches are ignored.

Table A-2. Radionuclide Data Sorted by Energy

Name	Energy	Desc	Yield (%)	Half Life	KUT	SGLS	HRLS
Pu-239	51.62		0.0271	24110 yrs		x	x
Am-241	59.54		35.9	432.2 yrs		x	x
Th-232	84.37	Ac-228	1.27	1.41E+10 yrs	x		
Np-237	86.48		12.4	4.761 yrs		x	
U-238	92.38	Th-234	2.81	4.47E+09 yrs	x		
U-238	92.8	Th-234	2.77	4.47E+09 yrs	x		
Pu-239	98.78		0.0012	24110 yrs		x	
Th-232	99.5	Ac-228	1.28	1.41E+10 yrs	x		
Eu-155	105.31		21.15	4.7611 yrs		x	
Eu-152	121.78		28.42	13.542 yrs		x	
Eu-154	123.07		40.79	8.593 yrs		x	
Th-232	129.07	Ac-228	2.45	1.41E+10 yrs	x		
Pu-239	129.3		0.0063	24110 yrs		x	x
U-235	143.76		10.96	7.04E+08 yrs		x	
U-235	163.33		5.08	7.04E+08 yrs		x	
Sb-125	176.31		6.82	2.758 yrs		x	
U-235	185.72		57.2	7.04E+08 yrs		x	x
U-238	186.1	Ra-228	3.5	4.47E+09 yrs	MDA		
U-235	205.31		5.01	7.04E+08 yrs		x	
Th-232	209.25	Ac-228	3.88	1.41E+10 yrs	x		
Th-232	238.63	Pb-212	43.3	1.41E+10 yrs	MDA	x	x
Th-232	240.99	Ra-224	3.97	1.41E+10 yrs	x		
U-238	241.98	Pb-214	7.5	4.47E+09 yrs	x		
Th-232	270.24	Ac-228	3.43	1.41E+10 yrs	x		
Th-232	277.36	Tl-208	2.27	1.41E+10 yrs	x		
U-238	295.21	Pb-214	18.5	4.47E+09 yrs	MDA	x	
Th-232	300.09	Pb-212	3.28	1.41E+10 yrs	x		
Np-237	300.34	Pa-233	6.62	1.41E+10 yrs		x	
Np-237	312.17	Pa-233	38.6	2.14E+06 yrs		x	x
Th-232	328	Ac-228	2.95	1.41E+10 yrs	x		
Th-232	338.32	Ac-228	11.25	1.41E+10 yrs	MDA	x	
Eu-152	344.28		26.58	13.54 yrs		x	x
U-238	351.92	Pb-214	35.8	4.47E+09 yrs	MDA	x	x
Pu-239	375.05		0.0016	24110 yrs		x	x
Th-232	409.46	Ac-228	1.94	1.41E+10 yrs	x		
Sb-125	427.88		29.6	2.7582 yrs		x	x
Th-232	463.01	Ac-228	4.44	1.41E+10 yrs	x		
Sb-125	463.37		10.49	2.7582 yrs		x	
Th-232	510.77	Tl-208	8.06	1.41E+10 yrs	MDA		
Th-232	583.19	Tl-208	30.11	1.41E+10 yrs	MDA	MDA	x
Sb-125	600.6		17.86	2.758 yrs		x	
Cs-134	604.7		97.56	2.062 yrs		x	x
U-238	609.31	Bi-214	44.79	4.47E+09 yrs	MDA	MDA	x
Ru-106	621.93	Rh-106	9.93	373.643 day		x	x
Sb-125	635.95		11.31	2.7582 yrs		x	
Cs-137	661.66		85.1	30.07 yrs	x	MDA	MDA
U-238	665.45	Bi-214	1.29	4.47E+09 yrs	x		
Sn-126	666.1		86	100000 yrs		x	x
Sn-126	694.8		82.56	100000 yrs		x	
Eu-154	723.31		20.22	8.593 yrs		x	x
Th-232	726.86	Ac-228	0.64	1.41E+10 yrs	x		
Th-232	727.33	Bi-212	6.58	1.41E+10 yrs	x		
Th-232	755.32	Ac-228	1.01	1.41E+10 yrs	x		
U-238p	766.36	Pa-234	0.29	4.47E+09 yrs		x	x
U-238	768.36	Bi-214	4.8	4.47E+09 yrs	x		
Th-232	772.29	Ac-228	1.5	1.41E+10 yrs	x		
Eu-152	778.9		12.96	13.54 yrs		x	

Table A-2. Radionuclide Data Sorted by Energy

Name	Energy	Desc	Yield (%)	Half Life	KUT	SGLS	HRLS
Th-232	785.37	Bi-212	1.1	1.41E+10 yrs	x		
U-238	785.91	Pb-214	0.85	4.47E+09 yrs	x		
Th-232	794.95	Ac-228	4.34	1.41E+10 yrs	x		
Cs-134	795.85		85.44	2.062 yrs		x	x
U-238	806.17	Bi-214	1.12	4.47E+09 yrs	x		
U-238p	811	Pa-234	0.51	4.47E+09 yrs		x	x
Th-232	835.71	Ac-228	1.68	1.41E+10 yrs	x		
Th-232	860.56	Tl-208	4.43	1.41E+10 yrs	x		
Eu-154	873.19		12.27	8.593 yrs		x	
Th-232	911.21	Ac-228	26.6	1.41E+10 yrs	MDA	x	
U-238	934.06	Bi-214	3.03	4.47E+09 yrs	x	x	
Th-232	964.77	Ac-228	5.11	1.41E+10 yrs	x		
Th-232	968.97	Ac-228	16.17	1.41E+10 yrs	MDA	x	
U-238	1001	Pb-214	0.84	4.47E+09 yrs	x		
U-238p	1001.03	Pa-234	0.84	4.47E+09 yrs		x	x
Eu-152	1112.12		13.54	13.54 yrs		x	
U-238	1120.29	Bi-214	14.8	4.47E+09 yrs	MDA	x	
U-238	1155.19	Bi-214	1.64	4.47E+09 yrs	x		
Co-60	1173.24		99.9	5.271 yrs		x	x
U-238	1238.11	Bi-214	5.86	4.47E+09 yrs	x		
Eu-154	1274.44		35.19	8.593 yrs		x	x
Co-60	1332.5		99.98	5.271 yrs		x	x
U-238	1377.67	Bi-214	3.92	4.47E+09 yrs	x		
U-238	1401.5	Bi-214	1.55	4.47E+09 yrs	x		
U-238	1407.98	Bi-214	2.8	4.47E+09 yrs	x		
Eu-152	1408.01		20.87	13.54 yrs		x	x
K-40	1460.83		10.67	1.28E+09 yrs	MDA	MDA	x
U-238	1509.23	Bi-214	2.12	4.47E+09 yrs	x	x	
Th-232	1588.21	Ac-228	3.27	1.41E+10 yrs	x	x	
Th-232	1620.5	Bi-212	1.49	1.41E+10 yrs	x	x	
Th-232	1630.63	Ac-228	1.6	1.41E+10 yrs	x	x	
U-238	1661.28	Bi-214	1.14	4.47E+09 yrs	x	x	
U-238	1729.6	Bi-214	2.88	4.47E+09 yrs	x	x	
U-238	1764.49	Bi-214	15.36	4.47E+09 yrs	MDA	MDA	
U-238	1847.42	Bi-214	2.04	4.47E+09 yrs	x	x	
U-238	2118.55	Bi-214	1.14	4.47E+09 yrs	x	x	
U-238	2204.21	Bi-214	4.86	4.47E+09 yrs	MDA	x	
U-238	2447.86	Bi-214	1.5	4.47E+09 yrs	MDA	x	
Th-232	2614.53	Tl-208	35.34	1.41E+10 yrs	MDA	MDA	

Notes:

- i. For natural radionuclides, all lines are associated with the parent radionuclide (²³⁸U or ²³²Th) and the half-life of the parent is given. The daughter radionuclide from which the gamma is emitted is indicated in the description column.
- ii. Yields for ²⁰⁸Tl are adjusted to account for the branching ratio (0.3594) for the decay of ²¹²Bi to ²⁰⁸Tl. All other branches are ignored.

Appendix B
Gamma-Ray Spectrum Analysis and
Concentration Calculation

Gamma-Ray Spectrum Analysis and Concentration Calculation

In gamma spectroscopy, individual gamma photons interact with the detector and generate electrical pulses with an amplitude proportional to the energy deposited in the detector. These pulses are sorted by amplitude and counted in individual “bins” or channels. For the logging systems commonly used at Hanford, 4096 channels are available. The raw gamma spectrum thus consists of a listing of counts in each channel number. During decay, many radionuclides of interest emit gamma photons at specific energy levels, which are a function of transitions within the atom. Although some radionuclides, such as ^3H , ^{90}Sr , or ^{99}Tc emit no useful gamma photons, others, such as ^{60}Co , ^{137}Cs , or ^{154}Eu emit one or more gamma rays at specific energy levels that are diagnostic of the presence of the radionuclide. Analysis of gamma spectra consists of identifying peaks in the raw spectra, establishing a relationship between channel number and energy level, identifying the radionuclide from the presence of diagnostic peaks, estimating background counts and net counts for each peak, and calculating the estimated or apparent concentration based on an assumed distribution and detector geometry.

The calculation is performed as a two-step process. In the first step, spectra analysis software is used to identify peaks and determine net counts. In the second step, an *Excel* workbook is used to calculate concentrations from the net count values. A brief description of the process, including specific format details and instructions for the *Excel* workbook, is presented below. Appendix C contains a more detailed discussion of the *Aptec* software used for spectrum analysis.

Spectrum Analysis Program

Gamma-ray spectra are acquired in the Ortec (*.CHN) format, and are analyzed with the Aptec Instruments Limited (Aptec) spectrum analysis program *PCMCA/WIN* (Aptec Instruments Ltd., North Tonawanda, New York); the version currently used is Version 6.3.1, Release 14. *PCMCA/WIN* can analyze the spectra in (*.CHN) format directly. Although spectra can be converted to the *Aptec* *.S0 format before analysis, using a program (*filecon.exe*) furnished by *Aptec*, the recommended practice is to keep the original spectra in Ortec (*.CHN) format, and to save processed spectra in *Aptec* (*.S0) format. Analysis results for processed spectra in *.S0 format, such as energy and resolution calibrations, and data for individual regions of interest (ROIs), are encoded in the spectrum files and preserved when the files are saved.

Three *PCMCA/WIN* analysis algorithms are used: *Peaksearch*, *Multifit*, and *Identify Peaks*. *Peaksearch* identifies features, called “regions of interest” (ROIs), that might be peaks by scanning a spectrum several times. The first scan simply seeks “statistically significant ‘bumps’ above background” (*OSQ/PLUS Installation and Operations Manual*, Rev. 01, p. 16, Aptec Instruments Ltd.), which are at least four multichannel analyzer (MCA) channels wide. A “bump” could be a full energy peak, an escape or sum peak, a superposition of two or more peaks, or high counts that happen, through statistical fluctuations, to occur in a set of four or more contiguous MCA channels. In subsequent scans, backgrounds for all ROIs are determined. A ROI background is represented by a polynomial function, up to fifth degree, that is fitted to counts in a number of “end channels” (channels on either side of the ROI that contain only

background counts). The degree of the polynomial is specified by the analyst, as is the number of end channels. The maximum number of channels on either side is 32. The software provides a provision to allow the number of end channels to vary linearly from one value at channel 0 to another value at the maximum channel. This feature allows the analyst to use fewer channels in low-energy regions where peaks are typically closer together.

If a small number of end channels is used for background fitting, the background determinations may be assisted by *Method 2*. If *Method 2* is invoked, background counts for channels *inside* the ROIs are estimated by linear interpolation and the background function is fitted using the estimated counts in channels inside the ROI, as well as counts from the end channels.

For each ROI, two quantities are determined. “Gross counts” is the sum of all counts accumulated in channels within the ROI. Background counts are the sum of background counts for channels within the ROI determined from the fitted background function. Each ROI is statistically tested as follows. The ROI percent error is calculated by

$$\text{percent error} = 100 \times \left(\frac{\sqrt{\text{gross counts} + \text{background counts}}}{\text{net counts}} \right) \times \sigma$$

(*PCMCA/SUPER Installation and Operations Manual*, Rev. 00, p. 47, Aptec Instruments Ltd.), in which the value of σ (“error sigma”) is entered by the analyst ($\sigma = 2$ has been consistently used). The maximum acceptable error value is specified by the analyst. ROIs with percent errors less than this criterion are accepted as peaks, while ROIs with greater errors higher are rejected. If *peaksearch* discards a ROI, the remaining ROIs are re-analyzed because of the possibility that the ROI rejection might affect the backgrounds functions for adjacent ROIs.

In the final spectrum scan, *Peaksearch* calculates the intensity of each ROI, in counts per second. An intensity is essentially the net counts (gross counts – background counts) for the ROI divided by the live counting time. *Peaksearch* also calculates the centroid, using one of several methods specified by the analyst. If a ROI corresponds to a full energy peak that is isolated, i.e., free of overlaps from other nearby peaks, then the centroid should be an accurate estimate of the peak energy and *Peaksearch* intensity should be an accurate estimate of the peak intensity, provided gamma intensity is not too high.

Peaksearch uses a statistical criterion to accept ROIs as peaks. It does not use the Mariscotti criterion or other shape analyzing techniques to attempt to distinguish true peaks from anomalous statistical features, nor does it attempt to determine if a ROI contains several superimposed peaks. ROIs are analyzed in more detail by the *Multifit* algorithm.

Multifit analyzes each ROI to look for evidence of multiple peaks within the ROI. Aptec’s *OSQ/PLUS Installation and Operations Manual* (Rev. 01, p. 23) states: “It has been shown that the best way of locating the centroids (centers) of overlapped peaks is by looking at the negative to positive crossing of the third derivative of the ROI. To compute the third derivative of the spectral data, one can cross correlate the spectrum with a filter function defined as the third derivative of a Gaussian distribution.”

After tentatively identifying peak centers within ROIs, *Multifit* performs the following test for each peak center candidate. The sum of counts for the 5 MCA channels centered on the candidate, minus the statistical uncertainty for the count sum, must be greater than the background for the same channels, plus κ (“MDA sigma”) times the background uncertainty. The value of κ can be set by the analyst, but the default value, $\kappa = 1.645$, has been consistently used.

For each peak center that is accepted, *Multifit* iteratively fits a Gaussian distribution function (GDF) to each peak adjusting parameters, and comparing the fitted results to the spectral data. The three GDF parameters that can be varied for peak fitting are centroid position, amplitude, and full width at half maximum (FWHM). Variations in the FWHM are usually constrained by a “resolution calibration,” which is a polynomial function (up to fifth degree) that relates the FWHM values to the MCA channel numbers of the corresponding peak centers. This can be “imported” from a previously analyzed spectrum, in which case the GDF fitting algorithm establishes FWHM values that are consistent with the imposed resolution calibration. If a resolution calibration is not imported, *multifit* will derive a resolution calibration using the FWHM values determined by the fitted GDFs. The program can display a plot of the FWHM values and the resolution calibration function, and the analyst can check the data for consistency with the usual trend; FWHM should gradually increase as peak energy increases. Wide ROIs may be fitted with several overlapping GDFs, which the Aptec manuals refer to as “multiplets.”

Gamma-ray sources are identified via the diagnostic gamma-ray energies. *PCMCA/WIN* calculates energies corresponding to peak centers expressed in MCA channel numbers using an energy calibration function. Like the resolution calibration function, an energy calibration function can be imported from a previously analyzed spectrum. If an energy calibration is not imported, it can be determined for any spectrum that has peaks for which the energies of the associated gamma rays are known. The *PCMCA/WIN* energy calibration feature allows the analyst to assign energies to the MCA channel numbers corresponding to the centers of such peaks. *PCMCA/WIN* then determines a polynomial (up to 5th degree) energy calibration function that relates MCA channel number to energy.

After *PCMCA/WIN* assigns an energy value to the centroid of every peak in a spectrum, the gamma-ray sources are identified by the *PCMCA/WIN Identify Peaks* algorithm. This algorithm compares each peak energy with entries in a library file that is essentially a list of radionuclides and gamma-ray energies. If the difference between the centroid energy and a library value is less than the specified tolerance, the peak is identified.

Obviously, the source radionuclide associated with a spectral peak will not be identified if there is no entry for that radionuclide in the library file. However, within the spectrum listing (*.LST) file, *PCMCA/WIN* will compile a list of unidentified peaks, with the associated energies and intensities. It is the responsibility of the analyst to survey the unidentified peak lists to determine if any previously undetected sources are present.

In logging practice, verification spectra are recorded at the beginning and end of each day with the sonde in a verification source containing known gamma lines with consistent intensity and

known geometry. Verification spectra are analyzed independently, and provide the energy and resolution calibration for analysis of log spectra.

Calibration

The gamma-ray source intensities can be calculated from the peak intensities (activities) via the detector calibration. The detector calibration equation is an energy-dependent function that relates peak intensity to the corresponding intensity of the source in the medium being logged, in gamma rays per second per gram. The source concentration can easily be calculated from the source intensity.

Data for determination of the calibration function are gained by logging four or more borehole calibration standards that contain known concentrations of the naturally occurring gamma-ray emitters, potassium (^{40}K), uranium (^{235}U and ^{238}U and their decay progenies), and thorium (^{232}Th and its decay progenies). DOE borehole calibration standards are large blocks of concrete that contain uniform distributions of potassium-, uranium-, and thorium-bearing minerals. Most of the blocks are right circular cylinders with a 4.5-in.-diameter test hole aligned along the cylinder axis. The following table displays source concentrations for the DOE standards that are customarily used (concentration data are from Steele and George [1986]). These standards reside at a Hanford calibration center located near the main entrance to the 200 West Area.

Source Concentrations for the Hanford Calibration Standards

Standard Name	^{40}K Concentration (picocuries per gram)	^{226}Ra Concentration ¹ (picocuries per gram)	^{232}Th Concentration (picocuries per gram)
SBK	53.50 ± 1.67	1.16 ± 0.11	0.11 ± 0.02
SBU	10.72 ± 0.84	190.52 ± 5.81	0.66 ± 0.06
SBT	10.63 ± 1.34	10.02 ± 0.48	58.11 ± 1.44
SBM	41.78 ± 1.84	125.79 ± 4.00	39.12 ± 1.07
SBA	undetermined	61.2 ± 1.7	undetermined
SBL	undetermined	324 ± 9	undetermined
SBB	undetermined	902 ± 27	undetermined
SBH	undetermined	3126 ± 180	undetermined

¹ Radium-226 is the fifth decay product of ^{238}U . If ^{226}Ra is in decay equilibrium with ^{238}U , then the concentrations (decay rates per unit mass) of the two nuclides are equal. The ^{226}Ra concentration is often cited instead of the ^{238}U concentration because most gamma-ray-based assays utilize gamma rays that originate in nuclides that are below ^{226}Ra in the uranium decay chain.

The source concentrations are expressed in picocuries per gram (which is actually activity per unit mass). A picocurie (pCi) is 10^{-12} of a curie, and a curie is 3.7×10^{10} decays per second, by definition.

For each source in a calibration standard, the product of the source concentration and the associated gamma-ray yield (number of gamma rays emitted per decay) is the source intensity, in gamma rays per second per gram. Gamma-ray yield values are published in nuclear data compilations, such as Firestone's *Table of Isotopes* (Firestone 1996).

In the case of ^{238}U , most of the “uranium” gamma rays originate not in ^{238}U itself, but in decay progenies, notably ^{214}Pb and ^{214}Bi , the eighth and ninth ^{238}U decay products, respectively. In the calibration standards, ^{238}U and its decay progenies exist in concentrations consistent with secular decay equilibrium, in which the decay rates of ^{214}Pb and ^{214}Bi are assumed to be equal to the decay rate of ^{238}U , and the source intensities for the ^{214}Pb and ^{214}Bi gamma rays can be calculated by multiplying the ^{214}Pb and ^{214}Bi gamma-ray yields by the ^{238}U concentrations.

Similar arguments apply to ^{232}Th . Most of the “thorium” gamma rays originate in ^{228}Ac , ^{212}Bi , and ^{208}Tl . With ^{208}Tl , it is also necessary to compensate for a branch in the decay chain: only about 36% of the ^{212}Bi decays to ^{208}Tl ; the remaining 64% decays to ^{212}Po , which then decays to ^{208}Pb .

Potassium, uranium, and thorium provide more than 250 gamma rays that are potentially detectable with the logging detectors. Of these, about 50 gamma rays spanning an energy range from 129.1 keV (^{228}Ac , thorium series) to 2614.5 keV (^{208}Tl , thorium series) have source intensities high enough to be useful for calibration. These source intensities have been calculated for all of the calibration standards.

The other data needed for calibration are spectral peak intensities. These can be acquired by logging the calibration standards and analyzing the spectra.

The value of the calibration function, $I(E)$, for a particular energy, E , is:

$$I(E) = \frac{\text{source intensity for the gamma ray of energy } E}{\text{spectral peak intensity for the gamma ray of energy } E}$$

For the first calibration, this equation was used to calculate values of $I(E)$ for many E values, then the $I(E)$ and E values were analyzed with a curve fitting program to determine a calibration function that could be used to calculate a value for $I(E)$ for any observable value of E . A calibration function of the following form was determined.

$$I(E) = (A + B \cdot \ln(E))^2.$$

To recalibrate, the calibration standards are logged, and the spectral peak intensities are determined and used to calculate revised values of the calibration constants, A and B , in the calibration function.

Source Concentrations

The concentration of a radionuclide is calculated as follows. The peak intensity is determined, then multiplied by the value of $I(E)$ for the particular energy. The product of $I(E)$ and the peak intensity is the source intensity, in gammas per second per gram. The source intensity is multiplied by the conversion factor, 27.027 picocuries per decay per second, and divided by the gamma-ray yield, in gammas per decay. The result is the source concentration, in picocuries per gram. That is, the concentration is

$$\text{concentration} = I(E) \cdot P \cdot \frac{27.027}{Y},$$

where P is the corrected peak intensity, in counts per second, and Y is the gamma-ray yield, in gammas per decay.

Peak Intensity Corrections

Hanford logging involves several instrumental and environmental effects that act to reduce spectral peak intensities. Calculated gamma-ray source concentrations would be erroneously low if corrections were not applied to offset these effects. Corrections for system dead time, borehole casing, and borehole water have been developed, and should be applied, when appropriate, to peak intensities before such intensities are used to calculate source concentrations.

Dead Time Correction

If a photon enters a detector and deposits energy, a brief signal processing time (usually around 10^{-6} sec) typically follows¹, during which the system cannot respond to additional photons that enter the detector. When the gamma-ray flux on the detector is high, significant numbers of photons go undetected, and the count rate is lower than would have been the case if every photon had been tallied.

Dead time typically is expressed as a percentage. It is calculated by:

$$DT(\%) = 100 \times (RT - LT) / RT$$

Where RT is the real time (clock time) over which the detector is operational, and LT is the live time, or time in which the detector is capable of generating counts.

SGLS dead time effects were characterized as follows. Small button ^{137}Cs sources were fastened near the detector inside the sonde. The flux of 661.6-keV gamma rays from these sources was constant (within statistical fluctuations) at the detector, but was not high enough to elevate the dead time beyond a few percent. Without disturbing the ^{137}Cs sources, the sonde was placed in the upper end of the test hole in the Department of Energy Grand Junction Office (GJO) U-1 calibration standard (uranium concentration = 7460 ± 465 pCi/g). Initially, the sonde was distant from the upper boundary of the uranium-bearing zone, where the dead time was low. Spectra were recorded as the sonde was incrementally advanced toward the uranium-bearing zone. Each movement of the sonde increased the intensity of the gamma-ray flux at the detector. As the radiation intensity increased, the percent dead time rose, and the intensity of the 661.6-keV gamma-ray peak decreased, even though the flux of 661.6-keV gamma rays was constant. The decrease of the 661.6-keV gamma-ray peak was attributed to dead time, and an empirical correction to offset the dead time effect was deduced.

¹ If the processing time is approximately constant in duration, the system is said to be “non-paralyzable.” If the processing time lengthens when additional photons enter the detector during processing, the system is “paralyzable.” The gamma-ray systems employed by DOE-GJO are non-paralyzable.

For the HRLS, dead time correction data were acquired in a similar manner, using point sources instead of a calibration model. A point source was moved incrementally closer to the detector to generate increasing gamma fluxes, and detector response to a source of constant intensity was monitored.

The dead time correction is

$$\text{dead time correction} = K_{DT} = \frac{1}{F + G \cdot T_D \cdot \ln(T_D) + H \cdot (T_D)^3},$$

in which T_D is the percent dead time and F , G , and H are constants. The correction is implemented by multiplying the measured peak intensity by the dead time correction.

Constants for the dead time correction function are dependent on the logging unit and type of system:

Logging Unit	F	G	H
SGLS Gamma 1A, 1B & 1D	1.0080	-4.71 E-4	-5.73 E-7
SGLS Gamma 2A & 2B	1.0322	-1.213 E-3	-1.89 E-7
HRLS Gamma 1C	1.033	-1.2 E-3	-1.6 E-6
RLS-1	1.03	-4.8 E-4	-4.8 E-7

Although the dead time correction was derived from data for the ^{137}Cs gamma-ray peak, additional investigations have shown that the correction is not limited to the 661.6-keV gamma-ray peak, but is applicable to peaks for all gamma-ray energies.

Steel Casing Correction

SGLS calibration functions are based on data collected by logging uncased holes. Obviously, the presence of steel casing reduces the observed gamma intensity, so application of the calibration to cased hole data would lead to underestimated radionuclide concentrations.

To offset the casing effect, an energy-dependent casing correction function has been determined. Casing correction data were recorded by logging the GJO KW Model² calibration standard (Steele and George 1986), then logging again with casing samples of various thicknesses mounted over the sonde. The casing correction at a particular energy E was defined as follows:

$$\text{correction at energy } E = \frac{\text{peak intensity for gamma energy } E \text{ from the uncased measurement}}{\text{peak intensity for gamma energy } E \text{ from the cased measurement}}$$

² The KW Model standard has potassium, uranium, and thorium distributed in a large rectangular block. The standard has five test holes with diameters of 3.0, 4.5, 7.0, 9.0, and 12.0 in. The sonde and sections of test casing could be placed in any of the three large-diameter holes.

Thus, if the value of the correction at energy E were known, the peak intensity from a cased hole measurement could be multiplied by the correction to derive the peak intensity that would have been recorded if the hole had not been cased.

A casing correction function for the SGLS was determined by combining measurements from both logging systems and using the averaged results to generate an energy-dependent casing correction function:

$$K_c = \exp\left(A_c + B_c \cdot E + \frac{C_c}{E}\right)$$

Where E is the gamma-ray energy, expressed in kilo-electron-volts, and A_c , B_c , and C_c are the fitting parameters. Each of the fitting parameters is related to the casing thickness, T . For T expressed in inches, the fitting parameters are:

$$A_c = -0.022 + 1.241 \cdot T$$

$$B_c = 1.17 \times 10^{-5} - 0.000213 \cdot T$$

$$C_c = 17.2 + 353.2 \cdot T$$

These values are applicable when the casing thickness is between 0.2 and 2.0 in., and for gamma-ray energies between 186 and 2615 keV. Care should be taken when extrapolating the casing correction to energy values beyond this range. Recent logging experience indicates the casing correction factor may be significantly low at 60 keV.

Water Correction

Calibration data were collected by logging uncased holes devoid of liquid. A borehole filled with water is occasionally logged. Obviously, water surrounding the sonde has an effect similar to that of casing, and a correction function is required to estimate radionuclide concentrations.

A correction function for water-filled holes was determined by logging four holes in the GJO KW Model standard. The hole diameters are 4.5, 7.0, 9.0, and 12.0 in. Each hole was logged without water and again with water; the sonde was centered for all measurements. The corrections were formulated similar to the casing corrections, i.e., a peak intensity from a water-filled hole measurement is multiplied by the correction to determine the intensity that would have been recorded if the water had been absent.

A water correction function for the SGLS was determined by combining measurements from both logging systems and using the averaged results to generate an energy-dependent water correction function:

$$K_w = \exp\left(A_w + B_w \times E + \frac{C_w}{E}\right)$$

Where E is the gamma-ray energy, expressed in kilo-electron-volts, and A_w , B_w , and C_w are the fitting parameters. Each of the fitting parameters is related to the hole diameter D. For D expressed in inches, the fitting parameters are

$$A_w = \left(1.406 - \frac{4.51}{D} \right)^2$$

$$B_w = \frac{0.00124}{D} - 0.000307$$

$$C_w = \frac{D}{0.168 - 0.0097 \times D}$$

These values are applicable when the borehole diameter is between 4 and 14 in., and for gamma-ray energies between 186 and 2615 keV. Because all of the water correction data were acquired with the sonde centered in the borehole (the cylindrical axis of the sonde coincided with the borehole axis), these water corrections are valid only for measurements acquired with the sonde centered.

Excel Workbook Instructions

The following discussion is included on the *Description* page of the *Excel* workbook for log data analysis. It provides specific details and operating instructions for calculating radionuclide concentrations from net count values.

Description of Log Analysis Spreadsheet

This spreadsheet is designed for routine calculation of concentrations from *.RAS files generated by *SGLSoffline*.

The spreadsheet is specific for a given system. The file name indicates the system and calibration date. G2BNov01.XLS is the correct workbook for SGLS Gamma 2B, using calibration data from November 2001. Calibration constants are built in. To modify the workbook for a different system or to update calibration, make the following changes:

- On the *I(E)* worksheet, change the calibration constants for I(E) in cells D13 and D14
- On the *DTC* worksheet, change the dead-time coefficients in cells B7, B8 and B9.

Worksheets *I(E)*, *DTC*, *Casing*, and *Water* are protected, except for cells where user input is allowed.

-  Indicates calibration data that should not be changed
-  Indicates areas where user input may be made when necessary

Summary Worksheet

The *summary* worksheet contains the borehole name, casing, and water data. This worksheet provides a common place where the analyst can input data that will be reflected throughout the workbook. Casing thickness values and depths are entered in the cells indicated. Casing thickness values are cumulative thickness for each interval.

Example: Outer casing 0.5 in. thick from 0 to 120 ft, with inner casing 0.25 in. thick from 0 to 240 ft and open hole from 240 to 250 ft.

Casing	Top	Bottom	T
1	0	120	0.75
2	120	240	0.25
3	240	250	0

If water is not a concern, enter "=NA()" in cell C8; any number in this cell will be taken as the depth to water

I(E) Worksheet

The *I(E)* worksheet contains the inverse efficiency calculation. This worksheet does not generally require user input. Concentration is calculated from peak counts per second by:

$$C_a(pCi/g) = \frac{27.027}{Y} * I(E) * K_c * K_w * P(cps)$$

Where Y is the radionuclide yield; I(E) is the calibration function; K_c and K_w are the casing and water correction factors; and P is the net count rate. The *I(E)* worksheet contains a table of energy and yield values for commonly encountered radionuclides in cells A17:C36. I(E) is calculated for each energy level in B17:B36 and displayed in D17:D36. For convenience, the above equation is simplified to:

$$C_a(pCi/g) = M * K_c * K_w * P(cps), \text{ where } M = \frac{27.027}{Y} * I(E)$$

The value of M is unique for each radionuclide energy, and accounts for the yield of that peak, as well as the calibration function. For a specific peak, such as the 661.62-keV gamma line for Cs-137, the value of M is constant. Yield values in C17:C36 are used to calculate specific M values, which are displayed in F17:F36. The name IE is assigned to the range 'I(E)!'\$B\$17:\$f\$36. Each individual radionuclide worksheet looks up the correct M value by energy level. A plot showing I(E) as a function of energy (E) is provided.

DTC Worksheet

The *DTC* worksheet contains the dead time correction function and generally does not require user input. Coefficients in cells B7, B8, and B9 are used to calculate specific dead time corrections on each radionuclide worksheet. A plot showing dead time correction as a function of % dead time is provided. Dead time corrections on the *0662HR* page are independently calculated using the function for the HRLS.

Casing Worksheet

The *casing* worksheet contains the casing correction function. The thickness values entered in cells D4, D5, and D6 on the *summary* worksheet should be reflected in cells C11, D11, and E11. In each column, the values calculated in rows 13, 14, and 15 are the coefficients for the casing correction function. Casing correction data are displayed in A17:E36. Radionuclide name and energy are reflected from the table on the *I(E)* worksheet to columns A and B. The casing correction coefficient is calculated as a function of energy level for each of three thickness values and displayed in columns C, D, and E. The name KC is assigned to the range 'Casing!'\$B\$17:\$E\$36. A fourth casing correction calculation is provided in column G for comparison purposes. Enter a casing thickness in G11, and corresponding casing correction coefficients will be calculated. A plot of casing correction as a function of energy is provided.

Water Worksheet

The *water* worksheet contains the water correction function. Depth to groundwater and borehole diameter are reflected from values entered on the *summary* page. The name KW is assigned to the range 'Water!'\$B\$21:\$C\$40. A plot of water correction as a function of energy is provided.

Radionuclide Worksheets (nnnn)

Concentration calculations for specific radionuclides are performed on these worksheets. The worksheet name indicates the energy of the peak. For example, "0609" indicates the Bi-214 peak at 609.31 keV. Columns A through G contain the input data (imported from the RAS file), and columns I through R contain the calculations.

Input columns

A	depth, ft
B	dead time, %
C	peak cps
D	cps unc (in percent)
E	MDA, cps
F	flag
G	filename

Analysis parameters

I1	Peak energy, keV	
J1	Bottom of 1 st casing interval	=Summary!C4
J2	Bottom of 2 nd casing interval	=Summary!C5
J3	Bottom of 3 rd casing interval	=Summary!C6
K1	Casing correction, 1st int	=VLOOKUP(\$I\$1,KC,2,0)
K2	Casing correction, 2nd int	=VLOOKUP(\$I\$1,KC,3,0)
K3	Casing correction, 3rd int	=VLOOKUP(\$I\$1,KC,4,0)
L2	Depth to groundwater	=Summary!C8
L3	Water correction	=VLOOKUP(\$I\$1,KW,2,0)
M2	Concentration coefficient (M)	=VLOOKUP(\$I\$1,IE,5,0)

Calculated columns

I	Error, cps	=Ci*Di/100
J	Dead time corr	=IF(Bi<10.5,1,1/(DTC!\$B\$7+DTC!\$B\$8*Bi*LN(Bi)+DTC!\$B\$9*Bi^3))
K	Casing corr	=IF(Ai<=J\$1,K\$1,IF(Ai<=J\$2,K\$2,IF(Ai<=J\$3,K\$3,NA())))
L	Water corr	=IF(SNA(L\$2),1,IF(Ai<L\$2,1,L\$3))
M	DTC*Kc*Kw*M	=Ji*Ki*Li*MS2
O	depth, ft	=Ai
P	conc, pCi/g	=IF(Ci<Ei,NA(),Mi*Cj)
Q	unc pCi/g	=Mi*li
R	MDL, pCi/g	=Mi*Ei

0662HR Worksheet

The page 662HR is for analysis of HRLS data and is valid only for Cs-137. The casing corrections are calculated from thickness values listed on the summary page. $M = 27.027 * I(E) / Y$ for the HRLS is included as a constant in cell M2. No water correction is available for the HRLS. Use column H for shield correction. Since the shield correction may vary from run to run, it should be entered manually in column H as the individual data are copied into the worksheet.

Input columns

A depth, ft
 B dead time, %
 C peak cps
 D cps unc (in percent)
 E MDA, cps
 F Flag
 G Filename
 H shield correction

no shield	ext shield	int shield	both shields
1	3.758	27.42	96.4

Analysis parameters

J1 Bottom of 1st casing interval ='Summary'!C4
 J2 Bottom of 2nd casing interval ='Summary'!C5
 J3 Bottom of 3rd casing interval ='Summary'!C6
 K1 Casing correction, 1st int =EXP(1.434*(summary!D4-0.28))
 K2 Casing correction, 2nd int =EXP(1.434*(summary!D5-0.28))
 K3 Casing correction, 3rd int =EXP(1.434*(summary!D6-0.28))
 M2 Concentration coefficient =3805.4 (Feb 2002 cal)

Calculated columns

I Error, cps =Ci*Di/100
 J Dead time corr =IF(Bi<10.5,1,1/(1.033-0.0012*Bi*LN(Bi)-0.0000016*Bi^3))
 K Casing corr =IF(Ai<=J\$1,K\$1,IF(Ai<=J\$2,K\$2,IF(Ai<=J\$3,K\$3,NA())))
 L not used
 M DTC*Kc*Ks*M =Hi*Ji*Ki*M\$2
 O depth, ft =Ai
 P conc, pCi/g =IF(Ci<Ei,NA(),Mi*Ci)
 Q unc pCi/g =Mi*li
 R MDL, pCi/g =Mi*Ei

grosscnt Worksheet

The *grosscnt* worksheet has gross gamma count data for the SGLS

Input columns

A	depth, ft
B	gross cps
C	true time, sec
D	live time, sec
E	dead time, %
F	gross counts

Calculated columns

H	Dead time corr	=IF(Ei<10.5,1,1/(DTC!\$B\$7+DTC!\$B\$8*Ei*LN(Ei)+DTC!\$B\$9*Ei^3))
I	Depth, ft	=Ai
J	DTC cps	=Hi*Bi
K	Dead time, %	=Ei

grosscntHR Worksheet

The *grosscntHR* worksheet has gross gamma count data for the HRLS

Input columns

A	depth, ft
B	gross cps
C	true time, sec
D	live time, sec
E	dead time, %
F	gross counts

Calculated columns

H	Dead time corr	=IF(Ei<10.5,1,1/(1.033-0.0012*Ei*LN(Ei)-0.000016*Ei^3))
I	Depth, ft	=Ai
J	DTC cps	=Hi*Bi
K	Dead time, %	=Ei

Plot Worksheets

The worksheets *GG&DT*, *MM*, and *KUT* contain pre-formatted plots that already reference the correct data columns. Each plot range is set for a total of 500 data points: if more points are required, the source data ranges must be extended manually. The Kc Plot worksheet contains a plot of casing correction factors for selected radionuclides as a function of depth. The plot helps the analyst check to ensure that the casing configuration is correct.

Transfer to *SigmaPlot*

To transfer data to *SigmaPlot* for final plotting, copy columns I, J, and K from the *grosscnt* worksheet and columns O, P, Q, and R from each radionuclide worksheet onto the correct columns on the *log data* worksheet. Use the paste special function to transfer the data as values. The *log data* worksheet can then be copied into *SigmaPlot*.

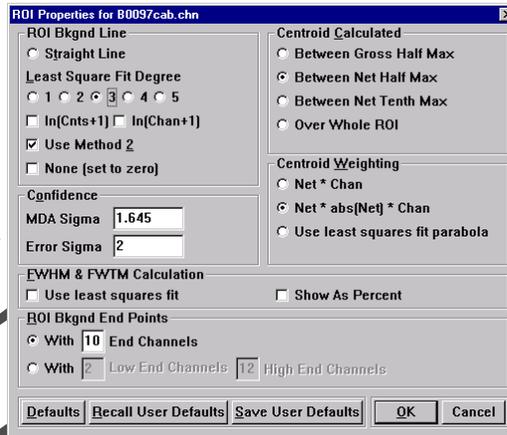
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Appendix C
User's Guide: Gamma Spectra Analysis
Parameters for Aptec Software

User's Guide: Gamma Spectra Analysis Parameters for ApteC Software

SETUP ROI PROPERTIES

The ROI properties screen is used to determine how various ROI values such as centroid, Full Width Half Max, Background rate, etc., are calculated. This screen is also accessible from the peak search screen because the choices made here affect the peak search.



ROI Bkgnd Line

The background line option offers the choice of a simple Straight Line fit between the end-point background averages, or a Least Squares Fit of either a first through a fifth order polynomial equation through the selected number of background channels on each side of the ROI. A first order fit is a straight line, a second order is a parabola, and a third order will allow an "S curve" type of fit. After the peak search, the ROI background line will be shown on-screen and all ROIs recalculated.

Use Method 2

Use Method 2 uses a straight-line background fit to estimate background values inside the ROI and includes these values in the regression to calculate fit parameters. This helps when using a small number of end points and a high-order fit. *[The final result is a least-squares polynomial fit of the specified order that will tend to be "flatter" through the ROI.]*

[Method 2 is a modified polynomial fit procedure that utilizes projected values inside the ROI to calculate the best background fit. Use of this method does not preclude specifying a large number of end channels. The only time a large number of end channels should not be specified is when there are multiple peaks adjacent to each other, and at most, a second order fit is being used.]

Centroid Calculated

Because a non-Gaussian peak will produce a weighted average centroid several channels in the direction of the "tail", options are provided to narrow the range over which the formula is applied.

Between Gross Half Max: Scans the peak from the channel with the highest count until it reaches the first channel below 1/2 value of the highest count or the lower limit of the ROI. It is assigned as the start channel. The ROI is then scanned right to determine the stop channel. The weighting formula is applied between the above determined start and stop channels.

Between Net Half Max: Derives the centroid between the channels previously determined to be the FWHM channels, rounded to the nearest integer channel.

Between Net Tenth Max: Derives the centroid between the channels previously determined to be the FWHM channels, rounded to the nearest integer channel.

Over Whole ROI: Derives the centroid using the lowest and highest channels in the ROI.

[Calculation of the centroid is not critical except for the energy calibration. In the energy calibration, the centroid channel is associated with the peak energy. If a peak has a large tail in one direction because of noise in the pulse line, the centroid could be slightly off, making the energy calibration error relatively high for that particular peak. This energy calibration error is not of great concern, but it is a wise practice to use the setting "Between Net Half Max." Then, for example, if the 2614-keV peak has a large tail, the centroid calculation will not be off by a significant amount.]

Confidence

MDA Sigma The larger this number is the more confidence there is in the MDA value reported. This also makes the reported MDA larger as a consequence.

Error Sigma All errors are multiplied by this value before reporting them on screen in print outs.

[Use 1.645 for the MDA Sigma. This is the 1-sigma (60% confidence interval) for the Aptec-calculated MDL. For the Error Sigma, use 2 (95% confidence interval).]

Centroid Weighting

The peak centroid of each ROI is calculated as a weighted average using either:

Net * Chan

Net * Chan = SUM (Net Count * Channel #) / SUM (Net Count)

$Net * abs(Net) * Chan$

$Net * abs(Net) * Chan = \text{SUM}(Net \text{ Count} * abs(Net \text{ Count}) * Channel) / \text{SUM} (Net \text{ Count} * abs(Net \text{ Count}))$

*[Select $Net * abs(Net) * chan$, although the difference will always be insignificant; this project uses 4000 channel spectra, and the peaks are defined by a large number of channels.]*

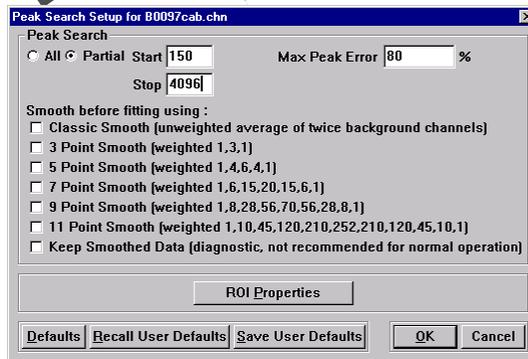
ROI Bkgnd End Points

With X End Channels: Where X is 0 to 32 channels on either side of the ROI used for fitting the background line. *[use 10 end channels]*

With X Low End Channels Y High End Channels: Where the number of end points is allowed to vary across the spectrum from X channels at the low energy end (channel 0) and Y channels at the high energy end (maximum channel number). This allows for peaks closer together in the X ray region of the spectrum.

PEAK CALCULATION SETUP

The multi-pass PEAK SEARCH is started by pressing P or from the ANALYZE pull-down menu. It should first be setup by pressing Shift P, or from the Peak Search item under the Analyze Setup sub menu.



Peak Search

All: Search all channels for peaks

Partial: Search between Start and Stop channels for peaks. This is useful when evaluating the various background fit methods. *[This feature is also useful for eliminating “noise” in the low-energy part of the spectrum.]*

[Use a partial-channel peak search and eliminate the low-energy photo-electric region from consideration, otherwise several noise peaks will be identified. Start the channel search at about

150 and stop at channel 4095. This will limit processing in the low-energy "knee" and truncate processing at the end of the spectrum.]

Max Peak Error: Only allow peaks with a Net Error * Error Sigma of less than Max Peak Error

[For verification spectra, start at about 50%. This setting should identify all the peaks tracked with the field verification spectra. If there is a problem with identifying peaks, the Maximum Peak Error can be increased. For routine analysis, a value of about 80% should be used.]

Smooth before fitting: Various options to smooth the spectrum before peak search

[Do not check any of the boxes listed.]

Methodology of the Peak Search

The multi-pass peak search routine first finds "peaks" using a rate of change of slope algorithm (similar to a first order derivative) and sets regions of interest (ROIs) around such areas. Next, the backgrounds around the ROIs are calculated using the end-points as per the setup feature. Then statistics are calculated for each ROI, and ROIs are rejected if they have statistical errors greater than the value set in the Peak setup. New backgrounds and statistics are recalculated as potential peaks are rejected. If the maximum of 256 ROIs have been set during any pass, the program halts, calculates backgrounds and statistics, and rejects peaks before continuing. ROIs that pass all criteria will then be considered as valid peaks.

TRICKS & TRAPS

Number of End Points

The number of end-points used in background averaging greatly influences the quality and speed of the peak search. The following guidelines may be used in optimizing the end-point averaging techniques for HPGe or Ge(Li) detectors. For NaI(Tl) use a small number (such as 0 to 4 end points) since the backgrounds are high and averaging does not enhance the results substantially.

- 1.) If backgrounds are high (at least several hundreds of counts per channel or above) and peaks are close, set the number of end points to be about 4-8 using a 1st order fit (for an 8K spectrum).
- 2.) If backgrounds are low (less than a few hundred counts per channel) and peaks are close, increase the number of end points to be in the range of 6-12 so that a better background statistics calculation can be made. For 4K or 16K spectrum, the number of end points used can be divided by 2 and multiplied by 2, respectively.
- 3.) If backgrounds are high and peaks far apart, the number of end points can be set as high as 32 and higher order background fits can be used. This mode would be employed to extract the highest accuracy during calibration.

- 4.) If backgrounds are low and peaks far apart, the number of end points should be between 10-20 channels.

Because of much higher counting efficiency and poorer resolution, the NaI(Tl) peak search error value should be set 5-10 times lower than for Germanium-based detectors (i.e., the error should be set to be between 10-50%).

Note: Use 2nd order (or greater) background averaging only when you have at least 10 end points.

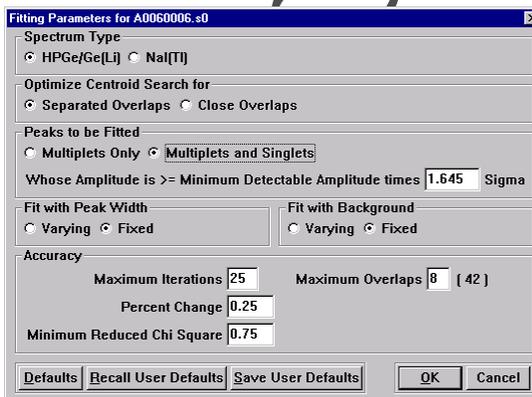
For hi-sensitivity, hi-accuracy peak location (i.e., to locate the maximum number of peaks) use 50-100 % 2 sigma error (N.B., 100% 2 sigma and 150% 3 sigma will give the same results as 50% 1 sigma).

In general, use the highest number of end points possible, up to the point where backgrounds do not properly follow the computer generated fit. This is most noticeable at low energies where peaks can be very close together and there are not enough clear points to properly define a background region.

Spectra that have peaks with poor counting statistics or very wide peaks MAY require smoothing before doing a peak search. Use one (or more) 7 or 9 point smooth on NaI(Tl) spectra before a peak search; a 3 or 5 point smooth will sometimes be useful with Ge or Si spectra.

MULTIFIT PARAMETERS SETUP

By running Multifit, all peaks will be fitted with a Gaussian distribution; the peak shape information determined from the verification spectra is used to calculate the experimentally determined Gaussian distributions in low count-rate spectra where the peaks have high uncertainties. In this manner the known response of the system is used to help determine an unknown quantity in another spectrum. This process helps to minimize the error of Gaussian fits of low-intensity peaks and is based on the assumption that the peaks are Gaussian distributions.



Spectrum Type

Choose the most appropriate from this option. NaI(Tl) spectra must be acquired with 256 or 512 channels, the routine will not attempt a fit if above this value. HPGe (and Ge(Li)) spectra can be successfully fit up to 16K channels.

Optimize Centroid Search for

Choose Separated Overlaps if all peaks in a multiplet can be very easily seen at their FWHM values or are even further apart. If this is not the case, use the Close Overlaps option.

Do not use the Close Overlaps option if there is severe tailing on the peaks or if you need the best possible signal to noise ratio for small peak analysis.

[Optimize Centroid Search for Close Overlaps may identify a tail on a larger peak as a separate peak. On the other hand, if the main peak is skewed or has an inappropriate shape, the number of counts in the peak will be questionable when a Gaussian curve is fitted to the peak. General practice has been to select Close Overlaps and delete any peaks that are clearly related to tails on the major peaks. If it is apparent that the counts in the tail peak should be included in the "main" peak, it may not be appropriate to try to fit a Gaussian surface to the peak. In this case use the identified ROI as the peak].

[Aptec 6.31 appears to do a better job of eliminating tail peaks when Separated Overlaps has been selected. The danger here is that overlapping peaks may not be identified. When processing log data, this is usually not a problem because there are only a few peaks in normal log spectra. Selection of Separated Overlaps will greatly reduce the labor required to edit a spectral data set.]

Peaks to be Fitted

Multiplets Only Fit only peaks determined to be multiplets

Multiplets and Singlets Fit all peaks

Whose Amplitude is \geq Minimum Detectable Amplitude Times **K** Sigma

The value that you enter here is the K value for the confidence levels for fitting. It is important that the fitting routine can make logical rejection or acceptance of peaks based upon statistical criteria. The default value of 1.645 represents a 95% confidence that the peak to be fitted is real.

[Multiplets and Singlets will fit all peaks with a Gaussian Distribution. This procedure uses the system's shape response[resolution calibration] to fit peaks with less than ideal count statistics, and therefore produces slightly lower error values. Set the Sigma values at 1.645.]

Fit with Peak Width

It is usually best to fit with the peak width fixed. The peak width is derived from the resolution vs. channel calibration curve. Use the Peak Width Varying option very carefully. A possible application would be if there had been a slight overall resolution broadening (of 5 % or so) and you were unable to re-calibrate.

[The “fixed” setting fixes the peak centroid to the shape calibration and will be the standard method of calculation. In this manner the peak shape information is used to help quantify the concentration. In some instances, it may be helpful to recalculate the multifit with the peak shape varying from the shape calibration. However, this recalculation would only be the case if it were necessary to minimize the error of a single peak that appears to have a significant tail because of system noise or some other cause. Be extremely careful about using a varying peak-width setting.]

Fit with Background

If the background is fixed, the background determined by the Aptec Application peak search is used as is. If allowed to vary then the ROI background equation is fitted with the Gaussian peaks to give the best overall fit. This will take slightly longer as there are more terms to vary.

[The “fixed” setting fixes the background so it does not change when the Gaussian fit is calculated and is not fine tuned for the Gaussian fit. Several spectra were checked to determine the difference between fixed and varying backgrounds for several peaks. Essentially no difference was found in any of the peak data. An error in earlier versions of Aptec resulted in an elevated background when this parameter was set to varying. Although the problem has been fixed, Aptec still recommends using the fixed background setting. Varying background should only be used for extremely high count rate data. This setting fixes the background to that which was calculated under the peak search routine. Attempts to optimize the background under the multifit routine will only introduce additional errors.]

Accuracy

Max Iterations: If the fit is not converging properly this will force the routine to stop after a certain number of iterations. A well-defined doublet with pure Gaussian peaks typically will converge in 4 or 5 passes. The default value of 20 is a good general-purpose number and should not have to be changed as there are other parameters that will make good fits stop faster.

Percent Change: As the fit converges properly, the change in the goodness of the fit will become less. Once a value of less than a 1% change per fit has been met, the fit will probably not get much better. The default value of 0.5% is a good general-purpose number.

Min Reduced Chi Square: Because a good fit is one for which the reduced Chi square is 1.0, and a reduced Chi square less than 1.0 does not indicate a better fit, the user can set the minimum Chi square value. This prevents the program from taking too long to converge or never converging at all.

If the Minimum Reduced Chi Square value is reached prior to either the Max Iterations or the Percent Change limits, the program will assume that the condition for convergence has been reached. At this time the program will move on to the next ROI and begin fitting it. It represents the difference between the fitted Gaussian at their calculated centroids and the actual data. This parameter is therefore a safety feature.

Maximum Overlaps: The Maximum Overlaps fixes the maximum number of peaks in a given region that can be fitted at once. The time taken goes up very rapidly with the number of peaks being fitted together. The default is 8, which was the value used in previous versions where this parameter could not be changed. Note that if the peak width and/or background are allowed to vary then the maximum will not be as high because the total number of terms is fixed to fit in a 64k segment.

[Use from 20 to 40 for the maximum iterations, even though the program will never cycle through this many iterations. There are no significant time constraints when using workstations equipped with Pentium processors. Use a 0.25% change and a chi square value of .75%. None of these statistical limits will impose a significant calculation time. Limit the maximum overlaps to 4 or 5. None of the peaks tracked in the field verification data are comprised of more than three separate convolutions. Even if a third convolution exists, it is usually the result of a misidentified tail.]

SETUP IDENTIFICATION

Identification Setup for B0097cab.chn

Library
Select N:\MACTEC-ERS\Analysis\Sgls.lib

Match ROI centroid energy with energy of isotope
 with a tolerance of \pm 3 keV
 with a tolerance of \pm 0.5 \times FWHM keV

Half Life Limit 7 Use to Reject

Fraction Limit 5 %

Allow Identification to create "Force MDA" ROIs
with an ROI width of 2.07892 times it's FWHM

Identify All ROIs
 Identify ROIs with a valid FWHM
 Identify ROIs with a valid FWTM

Defaults Recall User Defaults Save User Defaults OK Cancel

Library

Select the desired library from the list box.

Match ROI Centroid Energy with Energy of Isotope

Select fixed tolerance or tolerance based on width of peak (FWHM). For a fixed tolerance enter a value to be used as a +/- value for peak match. Numbers past 6 digits will be rounded-off. Make sure that the value range is consistent with the spectral energy range. For example, if using an Alpha library with a 2- to 5-MeV spectrum, the Energy Match value will be in MeV. Use a value much less than 10% of the full-scale spectrum range and consistent with the FWHM capabilities of the detector. For tolerance based on peak width the FWHM option (the default) will change the energy window to reflect the resolution broadening at higher energies. For HPGe or Ge(Li) detectors, a value between 0.5 and 1.0 is best. For NaI(Tl) detectors a value of 1.0 to 2.0 is best.

[Check the keV tolerance because an energy identification priority is used. The tolerance should be 3 or 4 keV. If the energy calibration is off for some reason, many peaks will be unidentified, thus immediately informing the analyst that something is wrong with the processing.]

Half Life Limit

A value for the half life can be entered as a reject criteria, typically between 7 (less than 1% of the Isotope will be left) and 10 (less than 0.1% left). This is used as a reject criteria only if there is no other means of identification AND the Use to Reject box has been checked. *[This feature is not used for analysis of spectral gamma logs]*

Fraction Limit

Before accepting a peak as a possible match to a certain isotope, S_Ident checks the active library to determine where any/all other lines for that isotope would be located. Those lines are then checked to see if there is an ROI (i.e. peak) at that location. If there is a match at the other energies, then the yield at that energy is added to the yield at the line in question. All potential lines are scanned and the sum of the yields is compared to the sum of ALL POSSIBLE on-screen lines for the candidate isotope. The ratio of the two sums is compared to the user entered Fraction Limit and if greater than or equal to the limit, that isotope is accepted as a possibility. If not, it is dropped. *[For spectral gamma logs, this feature is "turned off" by selecting a low value.]*

[The fraction limit is essentially turned off by entering a low number such as 5%. The Aptec software is not used for the assay; therefore, multiple peaks from the same isotope should not be compared. If a high number is entered in the fraction limit, some of the uranium and thorium peaks may not be identified.]

Allow Identification to Create Force MDA ROIs

Allows for ROIs to be set for isotope lines marked Force MDA even if they were not found. The MDA lines are read from the selected library. The width of the ROIs thus set is based on a

multiplier times the full width half maximum (FWHM). The default value of 2.07892 is what previous versions of S_Ident used and is equivalent to full width 20th max. It is suggested that a value of 2.55 times the FWHM is more appropriate as this gives 95% of the area of a Gaussian peak.

Peak Criteria for Identification

Choose All to accept a match to all peaks, regardless of their FWHM or FWTM resolution values. The way the FWHM values are calculated is to scan from the centroid both left and right until a data channel is found within the ROI that is below the background + half maximum. If both a high and low channel are found then the ROI is considered to have a valid FWHM. If either the high or low point is missing then the ROI is probably a multiplet and might not have the correct centroid energy.

The way the FWTM values are calculated is to scan from the centroid both left and right until a data channel is found within the ROI that is below the background + 1/10th maximum. If both a high and low channel are found then the ROI is considered to have a valid FWTM. If either the high or low point is missing then the ROI is probably a multiplet and might not have the correct centroid energy.

[Select Identify All ROIs, and ignore the other buttons in this box. This setting assures that the analyst and not the computer decides what a valid peak is.]

Aptec ROI Paint and Paint Edit

Select Header Menu Item, then choose ROI Paint or ROI Edit (must be indexed to an ROI).

Function keys F3-F6 are used to expand, contract, and/or shift an ROI. In the Paint ROI option, the mouse can be used to paint an ROI directly on screen.

When OK, select Set, Clear, or Cancel.

TIP: To quick paint an ROI move the mouse cursor to the left side of the ROI and press Ctrl key and click the mouse. Next move the mouse cursor to the right side of the ROI and press Ctrl key and click the mouse.

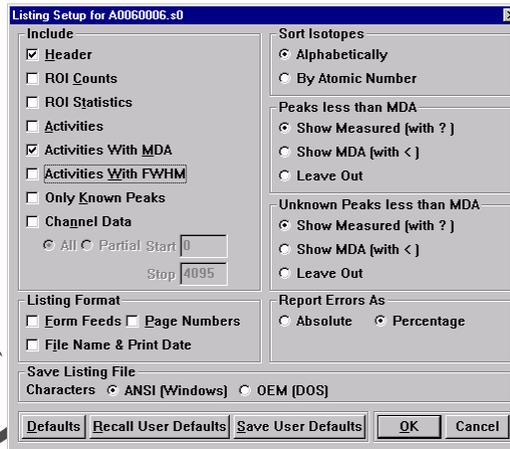
ROI Paint Menu

Delete	Delete an existing ROI being edited. Cancels the creation of an ROI being painted.
Cancel	Cancel edits to an existing ROI being edited. Cancels the creation of an ROI being painted.
Set (Ctrl-Click)	Accept the Painted ROI as shown.
<< >>(F3)	Expand the ROI one channel left and right.
>> <<(F4)	Shrink the ROI by one channel left and right.

<<--(F5) Shift the ROI one channel left

-->>(F6) Shift the ROI one channel right.

SETUP LISTING FORMAT



Include

<u>Header</u>	All header information.
<u>ROI Counts</u>	Raw data within regions of interest.
<u>ROI Statistics</u>	Precision of ROI data.
<u>Activities</u>	A concise qualitative and quantitative analysis format.
<u>Activities With MDA</u>	An expanded Activities format.
<u>Activities With FWHM</u>	An expanded Activities format.
<u>Only known Peaks</u>	Ignores peaks with energies not listed in the Library file
<u>Channel Data</u>	Choices include printing all channel data or partial (only channels in a region) channel data.

*[For verification spectra, select "Header" and "Activities with FWHM." When the listing is printed, this provides the information necessary to track the verification criteria. For spectral analysis, select "Header," "Activities with MDA," and "Activities with FWHM." Note that SGLSoffline reads these files to get the information for the *.RAS files. Depth is obtained from the "Sample ID" field in the *.S0 file.]*

Listing Format

Form Feeds: Advances to a new page for each portion of the printout. Leaving this blank will minimize the amount of paper that is used for a printout.

Page Numbers: Places sequential numbers on each printed page.

[Both "Form Feeds" and "Page Numbers" should be blank for spectral analysis].

Sort Isotopes

Alphabetically

Am-241 precedes Ba-133, Co-60, etc.

By Atomic Number

Uses an internal lookup table, Co-60, and Ba-133 precede Am-241.

Peaks Less than MDA

Show Measured (with ?)

Reports with a question mark (?) because they are less than the MDA.

Show MDA (with <)

Uses the < symbol to report.

Leave Out

Do not report if less than the MDA.

Unknown Peaks Less than MDA

Show Measured (with ?)

Reports with a question mark (?) because they are less than the MDA.

Show MDA (with <)

Uses the < symbol to report.

Leave Out

Do not report if less than the MDA.

[As a general rule, known (identified) peaks < MDA are reported with a ?, while unknown peaks less than the MDA are left out.]

Report Errors As

Absolute

Errors are in the same units as the quantified values.

Percentage

Report as a percentage value.

[Since the beginning of the baseline characterization project, errors have been reported as percentages. Even though it would appear to make more sense to report absolute errors, the percentage is still used for consistency with previous data.]

Energy Calibration

It is advisable to start the energy calibration with the highest energy (2614.53 keV) and then go to the lowest energy (186.1 keV) to cover the entire range of relevant energies. This approach will help to prevent confusion about what peak has been selected.

It is not absolutely necessary that the recommended peaks always be used for the energy calibration, but they are generally the most prominent in terms of peak to background and provide good coverage of the energy range of interest. The low (186.1 keV) and high (2614.53 keV) peaks must be used to ensure that the low- and high-energy calibrations are valid when using a third-order energy-to-channel fit.

If a mistake is made during the energy calibration, press F2 to clear the error, then redo the energy calibration beginning with the 2614.5-keV peak and continuing on with the 185.99-keV peak.

After the energy calibration is completed, view the energy calibration graph. Select Display, then Energy Calibration.

Choose Lin for the Display Scale (click on the scale descriptor in the upper left corner of the display). The curve should be fairly linear and a good spread and distribution of peaks should be displayed.

Change the display to Normal Spectrum, then select Full Energy Calibration under Setup to review the energy calibration statistics. The total energy calibration statistical error should be less than 0.1%. The 185.99-keV peak energy calibration error will be higher than any of the other peaks. If the statistics show a peak to be incorrect, go back to the spectrum display, index on the peak and erase it from the energy calibration (the energy calibration is displayed by pressing F2). This is accomplished by selecting the peak in the spectrum display and then deleting it (ROI, Delete Indexed). Replace the bad peak with the correct one, or correct the energy associated with the indexed peak.

Recommended Energy Calibration Points					
	Radionuclide	Energy		Radionuclide	Energy
1	Ra-226 (U-238)	186.10	9	Ac-228 (Th-232)	911.21
2	Pb-212 (Th-232)	238.63	10	Ac-228 (Th-232)	968.97
3	Pb-214 (U-238)	295.21	11	Bi-214 (U-238)	1120.29
4	Ac-228 (Th-232)	338.32	12	K-40	1460.83
5	Pb-214 (U-238)	351.92	13	Bi-214 (U-238)	1764.49
6	Tl-208 (Th-232)	510.77	14	Bi-214 (U-238)	2204.21
7	Tl-208 (Th-232)	583.19	15	Bi-214 (U-238)	2447.86
8	Bi-214 (U-238)	609.31	16	Tl-208 (Th-232)	2614.53

RESOLUTION CALIBRATION

When no resolution calibration has been performed, Multifit will perform it automatically. This is the preferred alternative, because it ensures reasonably consistent energy calibration among multiple analysts. In the event the automatic calibration does not seem sufficiently accurate, the following procedure is recommended.

To perform a resolution calibration, set the display to Normal Spectrum then select Full Resolution Calibration under Setup.

It will be necessary to input the ROIs. Select Edit Points, Load ROIs, OK-Fit.

Decrease the size of the full calibration window and return to the spectrum display window (by clicking on it) and display the Resolution Fit graph (Display, Resolution Calibration).

Delete bad (aberrant) peaks from the shape calibration. Aberrant peaks are identified from the statistical data and from the shape calibration graph. Toggle between the two displays to identify aberrant peaks (press Alt-Tab). Start by eliminating the peaks that have a statistically high positive error. Two energy peaks may be convolved together, producing a total sum peak that is interpreted by the program to be a single peak. These convolved peaks should be removed from the resolution calibration. In addition, peaks that are not primary photon peaks, (i.e., those that are the result of photon-detector interaction) should also be removed because they are too wide. Because of the physics of photon detection, it is best to eliminate all such extra wide peaks.

To delete a peak, double click on the appropriate line of text in the Full Resolution Calibration Display window; select Delete under Edit Points, then OK Fit.

Some peaks might interfere with the resolution calibration and should be deleted (e.g., 238, 511, 968, 1592, and 2103 keV).

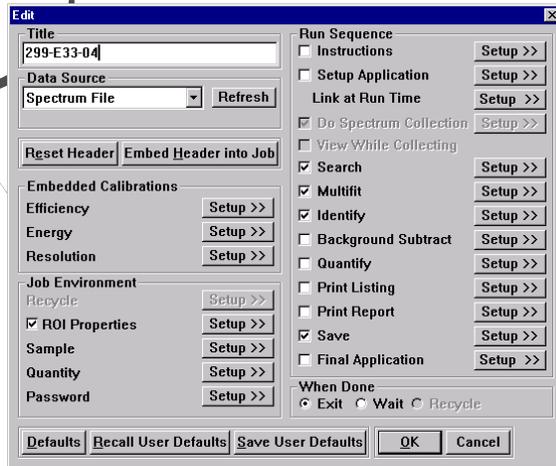
Some of the low intensity peaks may also cause problems when used in the shape calibration and should also be deleted (e.g., 328, 768, 836, and 1509 keV).

The 2614-keV peak may cause a problem. Because of noise in the spectrum, the peak may be too wide. Check the peak in the "normal" spectrum display (vertical split screen mode) to determine if it has a leading edge tail. Do not delete this peak from the shape calibration unless it is absolutely necessary in order to make the statistics reasonable.

Delete peaks from the shape calibration until the total error is about 3 or 4%. To avoid deleting too many peaks, assure that an adequate number of peaks are present for a meaningful second-order least squares fit, and that peaks are present at both ends of the spectrum. Typically, if there is a bad 2614-keV peak, the 2447- or 2204-keV peaks will help to produce an acceptable fit in the high-energy region of the spectrum.

When the shape calibration is satisfactory, close the Full Energy Calibration window, or select Exit under File and return to the spectrum display (Display, Normal Spectrum).

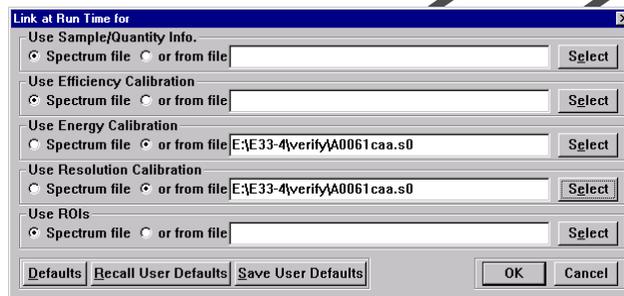
APTEC SUPERVISOR SETUP FOR BATCH PROCESSING



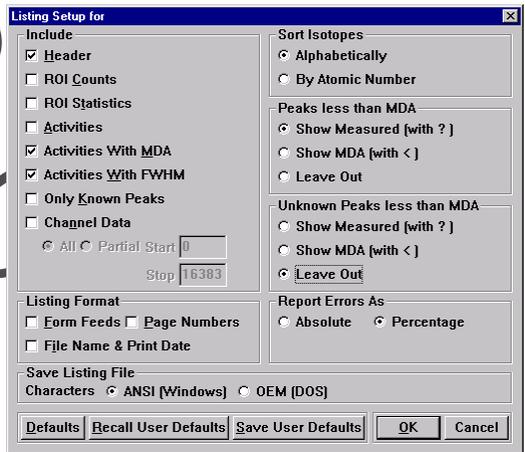
ROI Properties

see above

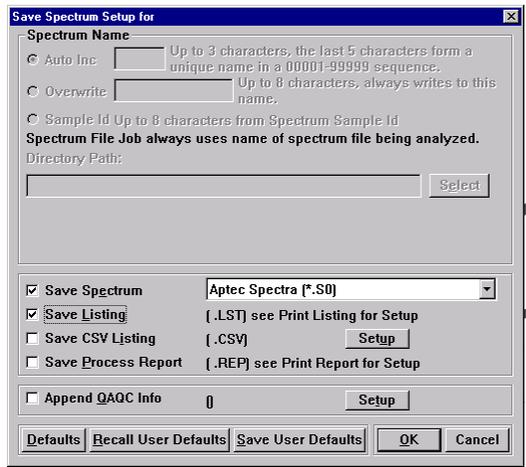
Link at Run Time



- Search see above
- Multifit see above
- Identify see above
- Background Subtract not used
- Quantify not used
- Print Listing Do not check, but use >>Setup to specify structure for file



- Print Report not used
- Save



- Final Application not used

Appendix D
Uncertainties in Log Data

Uncertainties in Log Data

After a spectrum is acquired and analyzed and a gamma-ray source is identified, the calculation of the source concentration involves the following steps:

- determine the spectral peak intensity
- apply the dead time correction
- apply the casing correction and any other environmental corrections
- multiply the corrected peak intensity by the value of the calibration function for the particular gamma-ray energy, multiply that result by 27.027, then divide by the gamma-ray yield

Each step involves quantities that have uncertainties. These uncertainties are all factored into an estimate of the experimental uncertainty for the source concentration. The uncertainty estimate is a measure of the precision (repeatability) of the calculated concentration.

The uncertainties in the various steps are calculated by methods that can be categorized as use of mathematical formulas, radiation counting methods, multiple identical measurements, and curve fitting.

Mathematical Formulas

Many quantities are calculated with formulas that involve measured quantities and their uncertainties. Uncertainties for such calculated quantities are estimated as follows.

If F is a quantity that is mathematically expressed in terms of M independent quantities, X_1, X_2, \dots, X_M ,

$$F = F(X_1, X_2, \dots, X_M),$$

the estimate of the 2σ uncertainty in F , or $2\sigma F$, is

$$2\sigma F = 2 \cdot \sqrt{\sum \left(\frac{\partial F}{\partial X_i} \cdot \sigma X_i \right)^2}.$$

This is a standard formula for the propagation of uncertainties. An example is provided by the casing correction. If the casing correction (at some particular energy) is K_C , and the peak intensity (for the same energy) is P , then the corrected peak intensity is $P \cdot K_C$. The expression for the uncertainty for the corrected peak intensity is derived as follows.

$$F(P, K_C) = P \cdot K_C$$

$$2\sigma F = 2 \cdot \sqrt{\left(\frac{\partial F}{\partial P} \cdot \sigma P \right)^2 + \left(\frac{\partial F}{\partial K_C} \cdot \sigma K_C \right)^2}$$

$$2\sigma F = 2 \cdot \sqrt{(K_C \cdot \sigma P)^2 + (P \cdot \sigma K_C)^2} = 2 \cdot \sqrt{\left(\frac{K_C \cdot P}{P} \cdot \sigma P\right)^2 + \left(\frac{P \cdot K_C}{K_C} \cdot \sigma K_C\right)^2}$$

$$2\sigma F = 2 \cdot \sqrt{\left(\frac{F}{P} \cdot \sigma P\right)^2 + \left(\frac{F}{K_C} \cdot \sigma K_C\right)^2} = 2 \cdot F \cdot \sqrt{\left(\frac{\sigma P}{P}\right)^2 + \left(\frac{\sigma K_C}{K_C}\right)^2}$$

Radiation Counting

Uncertainties for quantities that involve radiation counts, such as spectral peak intensities, are based on the fact that radioactive decay is a Poisson statistical process, and, consequently, a measurement that yields N counts has an estimated 1σ uncertainty equal to the square root of N . A spectral peak with N counts would have a count rate of N/t , where t is the live counting time, and an estimated 1σ uncertainty of $(\sqrt{N})/t$.

The actual calculation of a peak intensity uncertainty by *PCMCA/WIN* is more complicated by far because of background fitting, background subtraction, and the fitting of a Gaussian distribution function to the peak. Details are provided, albeit superficially, in the Aptec manual *OSQ/PLUS Installation and Operations Manual* (Rev. 01, pp. 31-45, Aptec Instruments Ltd.). The program is configured to calculate 2σ uncertainties.

Multiple Identical Measurements

Some quantities are determined from multiple identical measurements. An example would be a peak intensity used for calibration. For calibration, six or more spectra are collected from each calibration standard without changing any measurement conditions; therefore, each peak intensity is measured at least six times. The best estimate of any spectral peak intensity is the weighted average of the measurements. A weighted average and its associated uncertainty are calculated as follows.

If R_1, R_2, \dots, R_M are M measurements of the same quantity, and if each measurement R_i has an uncertainty σR_i , then the weighted average, $\langle R \rangle$, is

$$\langle R \rangle = \frac{\sum R_i \cdot w_i}{\sum w_i}$$

Each weight, w_i , is

$$w_i = \frac{1}{(\sigma R_i)^2},$$

and the uncertainty in $\langle R \rangle$ is

$$2\sigma\langle R \rangle = \frac{2}{\sqrt{\sum w_i}}$$

Curve Fitting

A plot of one logging parameter in relation to another often implies that an equation linking the two quantities can be derived. An example is the SGLS calibration function, $I(E)$, which varies with the gamma-ray energy, E , in a predictable way. The relationship

$$I(E) = (A + B \cdot \ln(E))^2,$$

(which is purely empirical and not derived from radiation transport physics) was established with the curve fitting program *TableCurve Windows* (Version 1.11, Jandel Scientific, San Rafael, California). In this example, the input to *TableCurve Windows* consisted of the values for E , the values for $I(E)$, and the normalized weights derived from the $I(E)$ uncertainties. (The uncertainties in the E values were assumed to be negligible.)

If the i -th experimentally determined $I(E)$ value had an uncertainty $\sigma I(E)_i$, then the weight was

$$w_i = \frac{1}{(\sigma I(E)_i)^2},$$

and the normalized weight was

$$\frac{w_i}{\sum w_j},$$

that is, the normalized i -th weight was the i -th weight divided by the sum of all weights.

TableCurve Windows presented a list of dozens of eligible functions, from which the particular form of the $I(E)$ function was selected. For the selected function, *TableCurve Windows* calculated the values for the constants, A and B , and the 95-percent confidence intervals for the values of A and B . The equations for these very involved calculations are stated, essentially without accompanying explanation, in pp. E-1 through E-6 of the *TableCurve User's Manual* (Jandel Scientific, San Rafael, California). Because the 95-percent confidence interval for the calculated value of A extended from $A - 2\sigma A$ to $A + 2\sigma A$, and similarly for B , the uncertainties in A and B could be deduced.

Summary

When log data are analyzed, methods described in this appendix are used to factor uncertainties from the following sources into the determinations of uncertainties for gamma-ray source concentrations:

- uncertainties in the gamma-ray source concentrations in the calibration standards
- uncertainties in the calibration measurements
- uncertainties in the correction measurements
- uncertainties in the logging measurements.

All concentration uncertainties are expressed at the 2σ level, corresponding to the 95-percent confidence interval.

As are other aspects of data analysis, the methods of determining uncertainties are under constant review. One concept presently under consideration is that the calibration standard source concentration uncertainties and the environmental correction uncertainties should be left out of the source concentration uncertainty determinations. This idea was prompted by several considerations. For one, the calibration standard concentrations and uncertainties have constant values. Similarly, values for the environmental corrections (for example, the 0.28-in.-thick casing correction for the 661.6-keV gamma ray) and uncertainties have been calculated, and are regarded as constants. The parameters in the gamma-ray source concentration calculations that have constant values do not affect the precision¹ of the results, but the uncertainties associated with those parameters make the uncertainties in the calculated source concentrations systematically higher. The somewhat enlarged “error bars” probably portray the accuracies of the source concentrations properly, but may be detrimental to evaluations for which the measurement precision is more important than the accuracy. For example, if a log yields a ¹³⁷Cs concentration at a subsurface point that is different from the concentration determined for the same point at an earlier time, contaminant migration might be indicated. The migration assessment would depend on measurement precision, not accuracy, and it would seem that the assessment would be helped if the error bars were reduced by deleting factors unrelated to precision from the uncertainty calculations.

¹ “Precision” is indicated by the standard deviation for a set of measurements. If a number of measurements give nearly equal values, the standard deviation is small and the measurements are precise. Precise measurements are not necessarily accurate. “Accuracy” refers to the agreement of the measured value with the “true” value.

Appendix E
Minimum Detectable Difference in Counts

Minimum Detectable Difference in Counts

Radioactive counts and count rates are subject to fluctuations that are related to the statistical nature of the decay process. When two count rates are compared, it is necessary to determine if the observed difference is statistically significant. The discussion below follows a method described by Knoll (2000, pp. 94-96).

N_1 and N_2 are total counts from two individual measurements acquired at different times. Both are taken to be estimates of the mean value of a Gaussian (normal) distribution at the time of measurement. The estimate for the standard deviation is assumed to be equivalent to the square root of the counts.

$$\sigma_N = \sqrt{N}$$

The count rates, R_1 and R_2 , are determined by dividing the counts by the live time. The count rate is also assumed to follow a Gaussian distribution, because $R = N/T$. The estimate of the standard deviation for the count rate is:

$$\sigma_R = \frac{\sqrt{N}}{T} = \frac{\sqrt{RT}}{T} = \sqrt{\frac{R}{T}}$$

The difference in count rates between the measurements should also follow a Gaussian distribution. If there is no actual difference in the two counts, then the true mean values for R_1 and R_2 are the same and:

$$\sigma_{\Delta R} = \sqrt{\sigma_{R_1}^2 + \sigma_{R_2}^2}$$

We need to define a critical level, L_1 , so that the probability of false positives is minimal. (A false positive is defined as incorrectly concluding that R_2 is greater than R_1) For a one-tailed normal distribution, there is a 95% probability that the mean from a random sample of R_2 will lie below the mean from a random sample of $R_1 + 1.645 \sigma$.

Also, $\sigma_{R_1} \approx \sigma_{R_2}$, so that:
$$\sigma_{\Delta R} = \sqrt{\sigma_{R_2}^2 + \sigma_{R_1}^2} = \sqrt{2} \times \sigma_{R_1}$$

Therefore:
$$L_1 = R_1 + 1.645 \times \sqrt{2} \times \sigma_{R_1} = R_1 + 2.326 \times \sigma_{R_1}$$

In the case where a real difference in activity exists, the true mean value for ΔR is >0 , and we need to define the minimum value of R_2 for which the probability of false negatives is minimal. (A false negative is defined as incorrectly concluding that R_2 is equal to R_1) If $R_2 = L_1$, the false negative rate will be 50 %, because a Gaussian distribution is symmetric about its mean. To ensure that 95 % of the values in the R_2 distribution lie above L_1 , we define L_2 so that:

$$L_2 = L_1 + 1.645 \times \sigma_{\Delta R}$$

also, $\sigma_{R2} \geq \sigma_{R1}$, so that: $\sigma_{\Delta R} = \sqrt{\sigma_{R1}^2 + \sigma_{R2}^2} \leq \sqrt{2} \times \sigma_{R2}$

$$L_2 = R_1 + 2.326 \times \sigma_{R1} + 2.326 \times \sigma_{R2}$$

L_2 defines the level above which there is a 95% probability that the count rates are different.

From above, $\sigma_R = \sqrt{\frac{R}{T}}$ therefore:

$$L_1 = R_1 + 2.326 \times \sqrt{\frac{R_1}{T_1}}$$

$$L_2 = R_1 + 2.326 \times \sqrt{\frac{R_1}{T_1}} + 2.326 \times \sqrt{\frac{R_2}{T_2}}$$

L_1 and L_2 define specific values against which R_2 can be compared to determine if the difference between R_1 and R_2 is statistically significant (at a 95-percent confidence level):

$R_2 < L_1$ The difference in count rates is not significant

$L_1 < R_2 < L_2$ The difference in count rates is ambiguous

$R_2 > L_2$ The difference in count rates is significant

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Appendix F
Assessment and Evaluation of Historical Log Data

Assessment and Evaluation of Historical Log Data

This section will be prepared and implemented at a later date.

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Appendix G
Discrimination Between Natural
and Man-Made Uranium

Discrimination Between Natural and Man-Made Uranium

Uranium-238 (^{238}U) decays to stable lead-206 (^{206}Pb) through 13 intermediate radionuclides by alpha or beta emission. There are several "branches" in the decay series where an atom may decay by either alpha or beta emission, but minor branches are not significant: greater than 99% of the decay activity follows the main path. During decay, ^{238}U emits only a few low-intensity gamma rays, which are not suitable for quantification by gamma spectroscopy. Detection and quantification of ^{238}U are actually based on measurement of gamma emissions from daughter radionuclides.

^{238}U has a half-life of approximately 4.5 billion years; activity levels will remain constant over the time frame of any investigative activity. Over time, activities of the daughter radionuclides will increase until a state of secular equilibrium is achieved, wherein decay activities of the various daughters are approximately equal to that of the parent. This condition will be achieved whenever the half-lives of the daughters are less than that of the parent, but the time required to reach equilibrium depends on the half-lives of the intervening daughters.

Naturally occurring uranium is assumed to have been undisturbed over geologic time, such that daughter radionuclides remain in close proximity and secular equilibrium has been achieved throughout the decay chain. It follows that the observed activity of a daughter would be equivalent to the activity of the parent. This assumption forms the basis for conventional spectral gamma logging, where ^{238}U concentration is typically calculated on the basis of gamma activity associated with ^{214}Bi and/or ^{214}Pb .

Processed uranium has been chemically purified, and daughter products have been removed, so that a state of secular equilibrium no longer exists. Because both ^{214}Pb and ^{214}Bi are located far down the decay chain and several of the intervening daughters have long half-lives, a long time period (on the order of a million years) is required for secular equilibrium to be re-established. Thus, it would be expected that any processed ^{238}U would contain negligible ^{214}Pb and ^{214}Bi . Only the first two daughters (^{234}Th and ^{234}Pa with half-lives of about 24 days and 1 minute, respectively) of the series would build up to reach equilibrium with their parent ^{238}U in a reasonable amount of time. The next daughter in the chain (^{234}U) has a half-life of 2.47×10^5 years.

The first daughter, ^{234}Th , emits a 92-keV gamma ray with relatively low yield. This typically cannot be detected by the SGLS. However, the 1001-, 811-, and 766-keV gamma rays emitted from ^{234}Pa can be detected by the SGLS. Of these, the 1001-keV gamma ray is the most intense, with a yield of about 0.008 gammas per decay. The yields of these gamma rays are so low that when uranium is present at typical natural background levels of a few picocuries per gram, these peaks are not detected in SGLS spectra. A peak corresponding to the 1001-keV gamma ray (with supporting peaks at 811 and 766 keV) indicates that ^{234}Pa is present in significant concentrations, from which it can be inferred that ^{238}U must also be present at significant concentrations, because ^{234}Pa would quickly decay away if it were not continuously regenerated by ^{238}U decay.

Both naturally occurring and processed uranium also contain ^{235}U . The activity of this radionuclide can be measured directly from a 185.7-keV gamma ray. This peak generally is not detected by the SGLS when uranium concentrations are at background levels. The combination of elevated count rates associated with the 186- and 1001-keV gamma rays is a reliable indicator that processed uranium exists in the subsurface.

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**Appendix H
Identification of Radon**

Identification of Radon

The presence of radon (^{222}Rn) presents a complicating factor in quantification of naturally occurring uranium. ^{222}Rn is the sixth daughter in the uranium decay series. It is an inert gas with a half-life of about 3.8 days. As a gas it is more able to migrate in the subsurface and is known to accumulate in boreholes. Radon daughters include ^{218}Pb , ^{214}Pb , and ^{214}Bi , which are the primary gamma-ray sources in the uranium decay series. These radionuclides tend to “plate out” on surfaces, including the inside of the casing and the logging sonde. Secular equilibrium with ^{222}Rn is achieved in a few hours.

When ^{222}Rn is present, the activities of ^{214}Pb and ^{214}Bi may be locally perturbed, such that the gamma measurements indicate an increase in natural uranium concentration. This discrepancy is often noticed when comparing data from separate log runs performed on different days. This apparent increase in ^{238}U concentration can occur even though there is no corresponding change in the ^{40}K and ^{232}Th activities, and there is no change in the verification spectra.

One key to differentiating between a radon anomaly and elevated natural ^{238}U is comparison of uranium concentrations determined from the ^{214}Bi lines at 609 and 1764 keV. ^{214}Bi deposited as a radon daughter is likely to be located inside the casing, either on the inside casing wall or the sonde itself. In either case, the gamma rays do not pass through the casing on the way to the detector. When uranium concentrations are calculated, an energy dependent casing correction is applied. If significant amounts of radon are present inside the casing, the correction will be applied to gamma fluxes unattenuated by casing, the effect will be to increase concentrations determined from the 609-keV gamma ray, relative to those determined from the 1764-keV gamma ray, because the 609-keV correction is larger than the 1764-keV correction. If significant concentrations of ^{137}Cs are present, however, the net counts for the 609-keV gamma rays may also be affected by downscatter from the 662-keV gamma ray.

If radon concentrations remain constant, decay equilibrium between ^{214}Pb and ^{214}Bi will be established in a few hours. However, radon concentrations in the borehole are likely to be continually changing, and log runs are generally completed in a few hours. Under secular equilibrium, activities of ^{214}Pb and ^{214}Bi will be equivalent to that of ^{222}Rn . However, ^{214}Pb occurs earlier in the decay chain, and its activity will increase faster than that of ^{214}Bi during the period before decay equilibrium is established. Under these conditions, net count rates for peaks associated with ^{214}Pb may appear to be elevated relative to net count rates for peaks associated with ^{214}Bi . Prominent gamma rays for ^{214}Pb occur at 352 and 295 keV. If these peaks appear to be elevated relative to the 609- and 1764-keV peaks associated with ^{214}Bi , the presence of radon may be indicated.

Evaluation of SGLS spectra from log events where elevated radon is suspected suggests that the 295-keV gamma ray is frequently detected when radon is present, and less frequently, if at all, in cases where radon does not appear to be present. (Typical log counting times are too short to resolve this gamma ray.) This suggests that detection of the 295-keV gamma ray may be diagnostic of the presence of elevated ^{222}Rn concentration.

The chance that a specific gamma ray will be detected is a function of its energy and its yield. For comparison purposes consider the 1764-keV ^{214}Bi energy peak with a yield of about 15 percent and the 295-keV ^{214}Pb with a comparable yield of about 19 percent. If both gamma rays originate from the formation, the 1764-keV gamma ray will undergo less gamma attenuation through steel casing and will normally be detected by the SGLS. However, the 295-keV gamma ray is rarely detected at normal counting times because of casing attenuation, which is greater at lower energy. Conversely, if the gamma rays originate inside the casing, the less energetic gamma ray at 295 keV is not attenuated by the casing, and is more likely to be detected.

The phenomena responsible for elevated concentrations of ^{222}Rn in a borehole are not completely understood. ^{222}Rn is continually produced in the formation from decay of its parent ^{238}U . The ^{222}Rn gas apparently migrates through the formation and accumulates in boreholes as a result of differential pressure caused by the lag between changes in barometric pressure, and air pressure in the pore space of the vadose zone.

If elevated radon exists in a borehole, it is impossible to distinguish the gamma counts originating from the formation from those originating inside of the casing, and it is impossible to determine reliable ^{238}U concentrations. ^{238}U concentrations determined from the higher energy ^{214}Bi peak at 1764 keV are probably more representative of the formation but the degree of accuracy is unknown.

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**Appendix I
Stratigraphic Correlation**

Stratigraphic Correlation

This section will be prepared and implemented at a later date.

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