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K-EDGE DENSITOMETER
(KED)

User Manual

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K-EDGE DENSITOMETER (KED)
USER MANUAL

by

James K. Sprinkle Jr. and Walter J. Hansen

ABSTRACT

In 1979, a K-edge densitometer (KED) was installed by the Safeguards Assay group from Los Alamos National Laboratory in the PNC reprocessing plant at Tokai-mura, Japan. It uses an active nondestructive assay technique, KED, to measure the plutonium concentration of the product solution. The measurement uncertainty of an assay depends on the count time chosen, but can be 0.5% or better. The computer hardware and software were upgraded in 1992. This manual describes the operation of the instrument, with an emphasis on the user interface to the software.

WELCOME TO THE K-EDGE DENSITOMETER

In this chapter, you will learn

• how this manual is organized,
• the measurement principles of the densitometer,
• how to start up the system, and
• guidelines for the menu operation.

GENERAL

This document describes the operation of the K-edge densitometer (KED). Other related manuals are the KED Hardware Manual, the KED Software Manual and manuals for the commercially available components and modules. Additional information, including the results of measurement campaigns and performance evaluations, is in the references.

AUDIENCE

This manual is divided into three parts:

- The first part (Chaps. 1 and 2) introduces you to the KED, provides an overview of the features, and tells you how to get started. The options in the short menu will be discussed. This includes how to request a measurement and how to print out the instrument's activity logs. It is written for the operators who use the instrument routinely.

- The second part (Chaps. 3 and 4) explains the options in the full menu. This part is intended for the instrument supervisor: the operator who is to be the resident expert. It discusses the available advanced options, which may require more knowledge for proper use. For example, you will learn to print and edit the parameter file and the calibration Option.

- The third part (Chaps. 5 and 6) contains the analysis physics and instrument settings. You will learn about calibration procedures and trouble shooting. It is intended to be a resource of additional information.

- There might be a README.KED file on the computer. This updates the documentation after the user manual has gone to print.

MEASUREMENT TECHNIQUE

The KED measures the concentration of plutonium solutions. It provides precise assays of solutions from 50 g/L to 500 g/L. The result is independent of the quantity of other elements in the solution, but the method requires that there be no suspended solids or bubbles. Two results are computed. They are equivalent for the typical product solutions from the Tokai-mura plant. The "extrapolated" result is better if there are large concentrations of other nuclear materials, such as 100 g/L of uranium.

The KED instrument measures plutonium concentration by monitoring the transmissions of two gamma rays that bracket the plutonium K-absorption edge. This is possible because in general the gamma-ray transmission through a fixed sample increases as the gamma-ray energy increases. However, when the increasing gamma-ray energy passes an absorption edge, the transmission abruptly decreases. The energy of these absorption edges is specific to each element. Selenium-75 provides a gamma ray of 121.1 keV and ^{57}Co provides a gamma ray of 122.1 keV; these bracket the plutonium K-edge at 121.7 keV.

The KED uses a peak fitting process with response functions to determine the intensities of the desired gamma rays. Self-calibration of the response function parameters is performed during the measurements with no sample present.

A ^{109}Cd source fixed to the detector head is used to monitor the effects of deadtime and pileup in the electronics. The Appendix describes the measurement physics and equations in more detail. Figure 1 is a line drawing of the measurement geometry.

MEASUREMENT PROCEDURE

An assay consists of two independent concentration measurements. The results must be consistent or else the sample is checked for bubbles and then measured a third time. Each concentration measurement requires the use of two gamma-ray transmission sources. Therefore an assay consists of either four or six data acquisitions. The self-diagnostics that the KED performs on each measurement are described in the appendix.

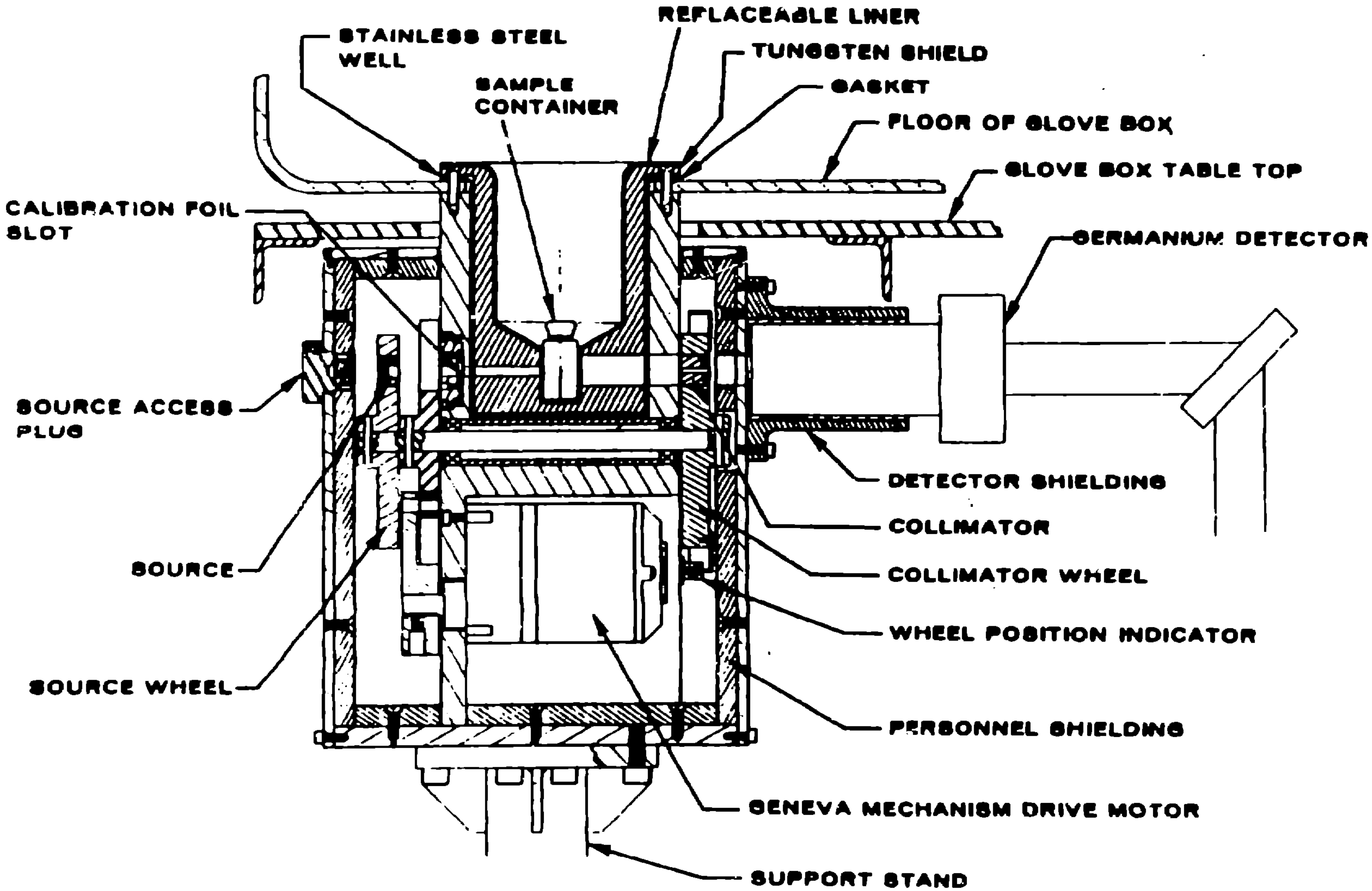


Fig 1. A line drawing (cross-section) of the K-edge Densitometer illustrates the measurement geometry. Important mechanical components such as the transmission source, sample container, and high-resolution detector are labeled.

MEASUREMENT PROCEDURE (cont.)

On a periodic basis, the intensity of the transmission sources is measured with no sample in the assay position. These "straight-through" measurements yield net peak areas that are used as the denominator in the transmission calculations. The straight-through measurements may be chosen to occur automatically each day at 00:00 hours or by operator request.

Additional periodic measurements are made to verify proper instrument response. These may be performed without a sample, or with stable, well-known items.

STARTING THE SOFTWARE

To recover from system halts or other severe problems, use the ctrl-alt-delete combination, or power the computer off for 10 s and then on again. The procedure to turn on the power is in the KED Hardware Manual.

The computer will automatically start the KED software when it is powered up. The start-up process takes 1 or 2 min. If the computer is not running the software, the KED software can be started by typing

CD\TOKAI[ENTER]
KED[ENTER],

The first screen on the CRT will be the one shown below.

```
                LOS ALAMOS NATIONAL LABORATORY

          K-edge Densitometer at Tokai-mura, Japan

                        Version 1.00

                  Release November 9, 1992


                Enter date (MM/DD/YY) 11/09/92

                Enter time (HH:MM:SS) 12:25:58

              Adjust the system Date if necessary
    [   ] to parameters   [F10] to save   [Esc] to cancel/exit
```

STARTING THE SOFTWARE (cont.)

The date and time can be adjusted if necessary. When the date and time are correct, push the F10 key. The computer will then initialize the Canberra S100 MCA.

Initialization

If the initialization of the computer-MCA communications is not successful, the operator is presented with the following *red* dialog box:

ERROR

MCA not responding
Continue without MCA operations Retry MCA connection Abort KED software Switch MCA Board number from 1 -> 2

Failure To Initialize

If the MCA cannot be initialized,

first, try a software reset: type ctrl-alt-delete. This will cause the system to reset the devices on the computer back plane and then restart the computer operating system.

second, try a hardware reset: power down the computer, wait 10 s, and power up the computer.

third, make sure the S-100 is configured correctly and seated in the back plane slot correctly.

The last choice, switching the MCA board number, is not used on this implementation. The KED uses MCA board no. 1.

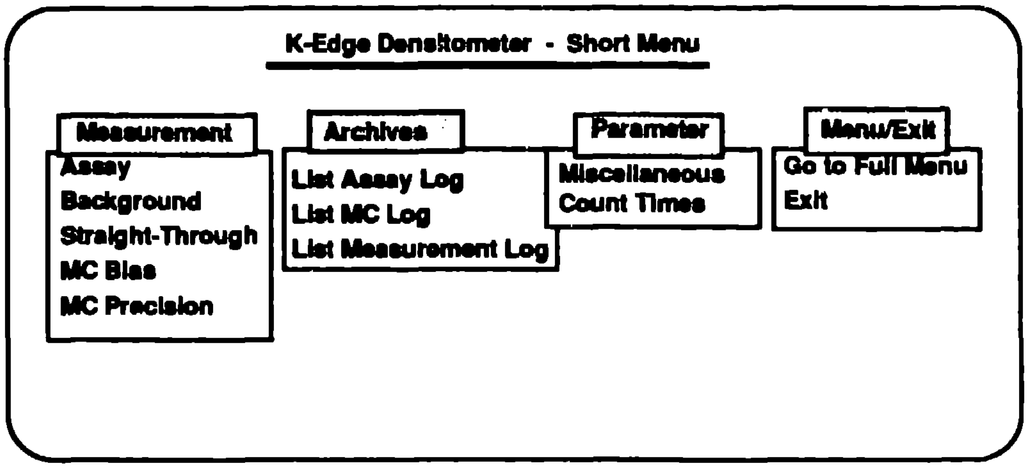
The program tries to initialize the printer; an error message appears if the printer is off or off-line.

If the data bases are not found, the software will create them and provide a warning message.

If the initialization is successful, the KED short menu will be displayed, as shown below. All routine operations can be

Failure To Initialize (cont.)

selected from this menu. The options in the short menu will be discussed in Chap. 2.



All other options of the KED system will be discussed in Chap. 3.

MENU OPERATION

The short KED menu is a pull-down-window format with four headings. The headings can be selected by pressing the "left" or "right" arrow key.

Option Selection

Under each heading there are several options that may be selected by using the "up" and "down" arrow keys to move the cursor to the desired option and pressing ENTER to activate the selected option.

Data Entry

Selecting an option displays a dialog box with the possible actions for the option. Defaults are built in with many of the inputs; a default response, if one is available, is listed in the blank after the question. The operator can modify the inputs.

Data Entry (cont.)

The operator may correct a response by using the "up" or "down" arrow key. The "home" key will bring the cursor to the top of the box; the "end" key will bring the cursor to the bottom of the box. Once the cursor is at the incorrect response, the operator can correct the response.

F10

When all the entries in the dialog box are correct, press F10 to have the computer accept the entries.

F2

The F2 function key is used to show the acceptable inputs of the highlighted entry. The "up" and "down" arrow keys can move the cursor to the desired input. The ENTER key will enter the input into the highlighted entry.

ESC

The operator can recover from incorrectly selected options with the ESC key. It will return the operator to the main menu so the operator may select an option.

To Stop an Assay

During the data acquisition, pressing ESC will bring up the following dialog box:

```
Assay suspended
Quit
Quit with Analysis
Resume Measurement
```

Moving the cursor to the appropriate option will enable the operator to quit or resume the assay.

During Data Entry

During data entry, the ESC key will bring up the following dialog box:

During Data Entry (cont.)

Warning

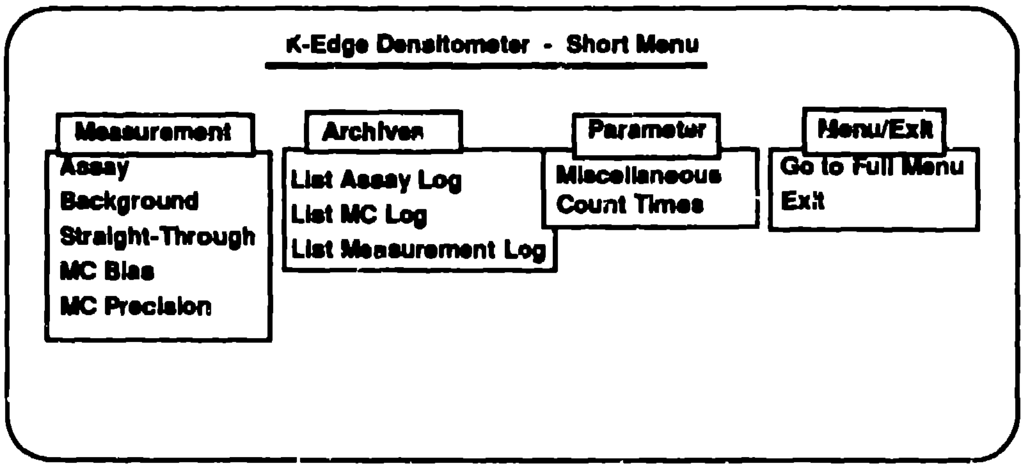
<ESC> is normally used to cancel all changes
Resume editing Cancel changes Save changes & exit form

Moving the cursor to the appropriate option will enable the operator to quit or cancel changes.

USING THE SHORT MENU

In this chapter you will learn about

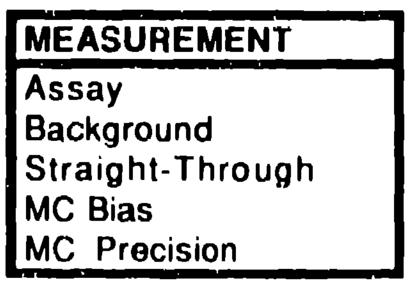
- Measurements
- Archives
- Parameters
- Menu/Exit



The short menu has four headings. These will be discussed in the next four sections.

MEASUREMENT OPTIONS

Five types of measurements can be made with the K-edge densitometer under the short menu. These will be discussed in the next five subsections.



To Stop a Measurement

During any data acquisition, pressing ESC will bring up the following dialog box:

Assay suspended
Quit
Quit with Analysis
Resume Measurement

After moving the cursor to the appropriate choice (Quit, Quit *with* Analysis, or Resume Measurement), pressing <return> will cause the selection to be activated.

Count Times

The precision of a computed result is dependent on the precisions of all of the measurements used to compute the result. Therefore, the count times used for the assay, straight-through, and background measurements all affect the precision of the assay. Better precision can be obtained with longer count times, up to a limit of ~0.3%.

Count times for the straight-through and background runs are used for each assay that follows them until those measurement types are repeated. This causes the results that share straight-through data to be correlated. Background effects and correlations are usually negligible for the Tokai-mura product solutions (>200 g/L).

Count times for the different measurement types are set in the parameter file. They can be changed in the edit option under the parameter heading in the full menu.

Assay

The Assay Option is used for the measurement of samples with an unknown plutonium concentration. Selecting the Assay Option displays the following dialog box:

Assay (cont.)

Assay Information
Operator:
Sample ID:
Remarks:

The user enters the operator and the sample identification. Up to 16 characters are allowed for the operator ID and up to 32 characters are allowed for the sample ID. The first eight characters of the sample ID are used to create the file name when spectral data are written to a disk file. Up to 40 characters are allowed for the remarks. If the information is not correct in any field, the user may use the arrow keys and the [delete] key and type the information again. When the information is correct, press F10 to proceed. Next, the software will ask the operator if the sample is in place, ready for measurement.

Count Time. It is recommended that the assay count time be shorter than the straight-through count time, unless the straight-through measurement is repeated before each assay. This will reduce the magnitude of the correlations between different assay results. The count time can be changed under the PARAMETERS Option (See page 33, the Count Time Option under the PARAMETERS Option in the chapter on the Short Menu.)

Measurement Results File. All results (peak areas, errors, etc.) from all measurements are automatically stored in the file

KED_DB.DAT

This file is to be distinguished from the raw data files that are discussed later.

Spectral Data File Name. If the Write Data to disk feature is selected (in the Default Option under the Parameter heading), two data files are written for each assay. The file name convention for each assay is

xxxxxxxx.Snn ^{75}Se source
xxxxxxxx.Cnn ^{57}Co source

where xxxxxxxx = first eight characters of the sample identification and

n = run number of assay.

The run number is automatically increased in increments of one to prevent overwriting previous data files with the same file name, for up to 99 files. The software will not check all output devices, this automatic increment will be applied to the first output device, which is expected to be the primary archive on the hard disk. If the Write Data to disk is selected, the hard copy printout will show the names of files written successfully to disk.

Display During Acquisition. While a measurement is in progress, the template that is seen on the computer display indicates the preset count time and the time remaining for that data acquisition. Some measurements require multiple data acquisitions. After the acquisition is finished, the display indicates which calculation is underway or if the printing to hard copy is active.

Sample Printout (Normal Output)

```
Tokai-mura K-Edge Densitometer                         NSB____________

                                                       IAEA___________

Sample ID: empty                          Measurement Type: ASSAY
Operator: James                           Measurement Date: 92.08.30
Remark:  let us try another output format
Straight-Through Date: 92.08.01           Constants File Date: 90.01.01
Live time (Se-75) = 60s                   Live time (Co-57) = 60s

                          Summary of Results
                        Pu concentration (g/ml)

Analysis method tested:   Simple

Cycle    Simple Method               Extrapolation
-------  --------------------        ----------------------

1        226.61624 +/- 2.85414       226.88812 +/- 2.83475
2        228.32866 +/- 2.76485       228.47076 +/- 2.74880

Average  227.55555 +/- 2.00000       227.55555 +/- 2.00000
Z1         0.90                        0.89

                     --- Assay Option PASSED ---
```

The *medium printout* will also include the net peak areas from each cycle, the disk filenames, and a header. The header includes the sample ID, the operator, the measurement date, and the count times.

Sample Printout (Normal Output) (cont.)

```
Tokai-mura K-Edge Densitometer                              NSB____________

                                                            IAEA___________

Sample ID: 123456789012                          Measurement Type: ASSAY
Operator: NAGANO                                 Measurement Date: 92.08.30
Remarks:
Straight-Through Date: 92.08.01                Constants File Date: 90.01.01
Data Files: 12345678.S01
            12345678.C01
            a:\subdirec\12345678.S01
            a:\subdirec\12345678.C01
            b:\oct92\subdirectory\12345678.S01
            b:\oct92\subdireccory\12345678.C01
Live time (Se-75) = 300s                          Live time (Co-57) = 288s

 Energy  Isotope    Net Peak Area          Normalized Area
-------  -------  ----------------------  ------------------
 88.036  Cd-109    158540.0 +/-   408.98   1.00000 +/- 0.00258
121.115  Se-75      44929.0 +/-   231.99   0.28339 +/- 0.00164
136.000  Se-75     163945.0 +/-   416.05   1.03409 +/- 0.00374

 Energy  Isotope    Net Peak Area          Normalized Area
-------  -------  ----------------------  ------------------
 88.036  Cd-109    150773.0 +/-   398.40   1.00000 +/- 0.00264
122.060  Co-57     909976.0 +/-   969.54   6.03540 +/- 0.01720

                                     Simple                 Extrapolated
                               ---------------------   --------------------
Calibration constant (cc/g)     6.12345 +/-  0.12345    6.12345 +/-  0.12345
Sample concentration (g/l)      1.11    +/-  1.49       1.06    +/-  1.42
```

Long Printout. The long printout is intended for diagnostic reports or troubleshooting. It prints the intermediate values from the calculations and the results of each diagnostic test.

Background

A background measurement is done with no sample in the measurement position and with both transmission sources in the shielded position. The background is computed for all of the peaks used in the instrument: the 88.036, the 121.115,

Background (cont.)

the 122.060, the 136.000, and the 279.528-keV gamma peaks. It also checks for a weak plutonium signal, using the 59.5-keV gamma ray from ^{241}Am and the 129.29-keV gamma ray from ^{239}Pu. A low background is important for assays of low-plutonium concentrations, but not for solutions of >150 g/L. Selecting the Background Option displays the following dialog box:

Background Information	
Operator:	
Sample ID:	BACKGROUND
Remarks:	

The user enters the operator identification as requested and any comments desired under Remarks. If the information is not correct, use the arrow keys and the [delete] key and type the information again. When the information is correct, press F10 to proceed. Next, the software will ask the operator to verify that the sample measurement chamber is empty: ready for the background measurement.

Recommended Frequency. This measurement technique is relatively insensitive to background. A background measurement should be done every 2-3 days, if solutions of low concentration (<150g/L) are to be measured.

Count Time. This measurement technique is relatively insensitive to background, but very short count times for the background measurement will affect the precision of the following assays. A minimum of 300 s is recommended for each background measurement.

Measurement Results File. All results (peak areas, errors, etc.) from all measurements are automatically stored in the file

KED_DB.DAT

This file is to be distinguished from the raw data files that are discussed later.

Warning Limit. The background count rates at selected gamma-ray energies are checked against a warning limit, which is stored in the parameter file. If a limit is exceeded, the corresponding warning message is printed in each assay that follows the background measurement. If this happens, the source of the background signal should be removed. The warning will remain in effect until the background measurement is repeated without failing the diagnostic test.

Spectral Data File Name. If the Write Data To Disk feature is selected (in the Default Option under the Parameter heading), the file name will be of the form

BCYYMMDD.Bnn

where YY = year,
MM = month,
DD = day of the month, and
nn = run number.

Display during Acquisition. While a measurement is in progress, the template that is seen on the computer display indicates the preset count time and the time remaining for that data acquisition.

Sample Printout (Normal)

```
Tokai-mura K-Edge Densitometer                      NSB____________________

                                                    IAEA___________________

                                              Measurement Type: BACKGROUND
Operator: Sprinkle                              Measurement Date: 92.09.30
Remarks:  This is the operator's remarks.
                                            Constants File Date: 92.09.28

Data Files: None
Live time (Blank) = 60s

                    --- Background Option PASSED ---
```

The medium printout will also include the net peak areas. The long printout will also include the results of the diagnostic tests.

Straight Through

A straight-through measurement is done with no sample in the chamber and with a data acquisition from both transmission sources. The results will be combined with the measurement results from succeeding samples to compute the sample transmissions for each. The 88.036-keV gamma ray is again used to normalize the other gamma-ray intensities to correct for dead time and pileup effects. Selecting the Straight-Through Option displays the following dialog box:

Straight-Through Information	
Operator:	
Sample ID:	Straight-Through
Remarks:	

Straight Through (cont.)

The user enters the operator identification as requested and any comments desired under Remarks. If the information is not correct, use the arrow keys and the [delete] key, and type the information again. When the information is correct, press F10 to proceed. Next, the software will ask the operator to verify that the sample measurement chamber is empty, ready for the straight-through measurement.

Recommended Frequency. A straight-through measurement is required at regular intervals. The maximum time allowed between straight-through measurements is adjusted in the parameter file. The frequency of straight-through runs is daily or weekly. The software has the capability to automatically initiate a straight-through measurement each day at 00:00 hours. This allows long count times when the instrument is normally idle.

Count Time. The precision of the straight-through measurement is more important than the frequency with which it is done. Results from the straight-through are used for each assay that follows them until the Straight-Through Option is repeated successfully. Therefore the results that share straight-through data are correlated. Each straight-through measurement should be run for a long time so that its statistical precision does not contribute significantly to the statistical precision of the transmission measurement used to compute an assay result. The straight-through run should be conducted for at least 1000 to 2000 s for both sources.

Count times for straight-through runs are set in the parameter file. They can be changed in the Edit Parameter Option.

Measurement Results File. All results (peak areas, errors, etc.) from all measurements are automatically stored in the file

KED_DB.DAT

This file is to be distinguished from the raw data files, which are discussed later.

Warning Limits. The normalized count rates from the 121.1-keV gamma ray (^{75}Se source) and the 122.1-keV gamma ray (^{57}Co source) are compared to the rates obtained in the previous Straight-Through measurement, with a correction for the half-life decays. If the rates are consistent, the limit is passed. If the rates are not consistent, a warning is printed that specifies the offending source, and successive measurements will include a repetition of that warning. Note that the ^{109}Cd will affect both transmission source normalized rates. After any new source is installed, ^{109}Cd, ^{75}Se, or ^{57}Co, two successive straight-through measurements will reset the expected value and confirm it.

Spectral Data File Name. If the Write Data To Disk feature is selected (in the Default Option under the Parameter heading), the file name will be of the form

STYYMMDD.Cnn
STYYMMDD.Snn

where YY=year,
MM = month ,
DD = day of the month,
C or S denotes the ^{57}Co or ^{75}Se source respectively, and
nn = run number.

Sample Printout (Normal)

```
Tokai-mura K-Edge Densitometer                          NSB_________

                                                        IAEA________

                                  Measurement Type: STRAIGHT-THROUGH
Operator: Willie                     Measurement Date: 92.09.30
Remarks:
                                      Constants File Date: 92.09.28

Data Files:None
Live time (Se-75) = 60s                  Live time (Co-57) = 60s

              --- Straight-Through Option PASSED ---
```

The medium printout will also include the net peak areas. The long printout will also include the results of the diagnostic tests.

MC-Bias

A measurement control–bias run is done regularly as part of the measurement control program. This measurement can be done with a plutonium foil, a plutonium sample, or a tantalum foil. The use of a tantalum foil for both transmission sources will provide a result that is very nearly zero. But placing a thicker tantalum foil into the transmission beam for the ^{57}Co source can simulate a plutonium assay. The following dialog box is presented after the MC–Bias Option is selected:

MC-Bias Information	
Operator:	
Sample ID:	
Remarks:	

MC-Bias (cont.)

The operator must select one of the sample ID's that have been previously set up in the parameter file. Use of the F2 button will suggest what choices are available.

After the measurement, the assay result is compared with a reference value stored in the parameter file. The same result (simple or extrapolated) is used for this test as has been selected for the bubble test. (See the Assay Criterion parameters in Chap. 4 - EDIT PARAMETERS.) The difference between the assay result and the reference value (in units of the historical standard deviation of the measurement) is compared to warning and action limits. If the warning limits are not passed, subsequent assays are accompanied by a warning in the results. If the action limits are not passed, further use of the Assay Option is not allowed until the MC–Bias Option is executed successfully. A negative value for the historical standard deviation will turn this test off. Five reference values are stored in the parameters, each with a sample ID.

Recommended Fre ency. An MC–Bias measurement is required at regular tervals with the maximum time allowed between bias runs being set in the parameter file. A single MC–Bias measurement of one of the reference items is recommended to be done weekly during periods of heavy use of the densitometer. otherwise we recommend that a single MC--Bias measurement precede any sample measurements after the densitometer has been idle.

Count Time. The count times are stored in the parameter file. They can be changed using the PARAMETER Option. The count times should be similar to those used for routine assays.

Reference Value. The assay result of an MC–Bias sample may not be the same as its actual plutonium content because the sample geometry is different from that of a solution. Therefore, the foil should be measured very precisely after every calibration and the reference value in the parameter file should be updated. Over a period of time (several years) the equivalent value of the foil may be known. The

Reference Value. (cont.)
measurement result will be directly affected by a change in the calibration constant. Both foils should be checked this way.

Historical Standard Deviation. The historical standard deviation of the foil data is determined by examining results obtained over extended periods of time. It should include all contributions that affect the assay with the exception of variations in sample depth and sample-vial variations. This precision will vary slowly with time as the transmission sources decay.

Warning and Action Limits. The difference between the MC–Bias assay result and the foil reference value, in units of the historical standard deviation, is compared against warning and action limits, assuming normal distribution. These limits can be adjusted in the parameter file under the Measurement Control Option.

Limit	Probability of Not Exceeding Limit
±1.00 std dev	0.6826
±1.96 std dev	0.9500
±2.00 std dev	0.9544
±3.00 std dev	0.9972
±4.00 std dev	0.9999

This test is sensitive to how well the historical standard deviation is known. If the proposed standard deviation does not include all long term and systematic errors, this test will fail more often than suggested by the table. An error of 30% in the historical standard deviation can change the results from the 4-σ level to the 3-σ level.

Spectral Data File Name. If the raw data are written to disk, the file name will be of the form

Spectral Data File Name (cont.)

MBYYMMDD.Snn
MBYYMMDD.Cnn

where YY = year,
MM = month of year,
DD = day of the month,
C or S denotes ^{57}Co or ^{75}Se respectively, and
nn = run number.

Sample Printout. The printout is the same as that used for an ASSAY, except that the Measurement Type is MC–Bias, and a message is printed at the very end of the printout stating whether the MC–Bias run PASSED or FAILED.

```
Tokai-mura K-Edge Densitometer                                NSB______________

   IAEA_____________

Sample ID: Ta_7_7                                     Measurement Type: MC-BIAS
Operator: Walt                                      Measurement Date: 92.08.30
Remarks:  <up   to   40   characters allowed>
Straight-Through Date: 92.08.01                   Constants File Date: 90.01.01
Data Files: None
Live time (Se-75) = 500s                               Live time (Co-57) = 650s

      Simple                        Extrapolated
                            -------------------     ----------------
Calibration constant  (cc/g)  6.12340  +/- 0.00120    6.43210 +/-  0.00210
Sample concentration  (g/l)   200.00   +/- 20.00     222.22    +/- 22.22

                                 MC-Bias Test

Analysis method tested:     Simple

                       --- MC-Bias Option PASSED ---
```

The medium printout will include the net peak areas. It will also include the measured result, the expected result, and the historical standard deviation.

Sample Printout (cont.)

If the MC–Bias test fails the WARNING or ERROR limit, a message stating the test information is printed. The LONG PRINTOUT is for diagnostic purposes. It includes the measured and expected values of all diagnostic tests.

MC–Precision

A measurement control–precision run is done regularly as a part of the measurement control program. This measurement can be done with any sample or an empty chamber. The measurement consists of multiple runs as specified in the parameter file. The assay results from these runs are analyzed statistically to verify that the random variations observed are consistent with those predicted from counting statistics. The test can fail in two ways. The first mode of failure is when the calculated variance propagated from counting statistics is incorrect. The formulas for these errors have been thoroughly tested, and we do not believe that this potential source of failure is present. The second failure mode will be because of instabilities in the counting electronics. This is indicated when the observed measurement variance from repeated runs is larger than the propagated variance.

Recommended Frequency. A measurement control–precision sequence is required at regular intervals with the maximum time allowed between sequences being set in the parameter file. A measurement control–precision run sequence should be carried out monthly. This test may be turned off by selecting a negative value for the frequency in the Edit Parameter Option.

Count Time. The count times for the ^{75}Se and ^{57}Co data acquisitions are set in the parameter file.

Number of Runs. The number of runs is set in the parameter file. Allowed values will be displayed when the operator presses the F2 button. The selection is restricted because the limits on the chi-square test depend upon the number of cycles. In general, a small number of short count time

Number of Runs (cont.)
measurements can pass the statistical tests more easily. A large number of long count-time measurements is a more stringent test.

Warning and Action Limits. The standard deviation of the replicate measurements is compared to the standard deviation estimated from the counting statistics of a single run. The value of the resulting chi-square/degree of freedom is tested against warning limits at 95% confidence and action limits at 99% confidence. These limits are fixed in the software. Failure of the warning limit will cause a warning to be printed for every succeeding measurement type, until the MC–Precision Option is successfully passed. Failure of the action limit will cause the system to not allow assays until the MC–Precision Option is successfully passed or a warning limit level is achieved. This test may be avoided by selecting a negative time for the repetition rate.

Spectral Data File Name. If the raw data are written to disk, the file name will be of the form

MPYYMMDD.Snn
MPYYMMDD.Cnn

where YY = year,
MM = month,
DD = day of the month, and
nn = run number.

Sample Printout (Normal)

```
Tokai-mura K-Edge Densitometer                                NSB______________

                                                              IAEA_____________

Sample ID: Ta7_7_7_7_7                      Measurement Type: MC-PRECISION
Operator: James                                 Measurement Date: 92.08.30
Remark:
Straight-Through Date: 92.08.01               Constants File Date: 90.01.01
Live time (Se-75) = 60s                             Live time (Co-57) = 60s

                         MC-Precision Test Summary

Number of measurements: 6
                                 Simple                Extrapolated
                            ------------------       ---------------
   Average result (g/l)      200.00                  222.22
   Standard Deviation (g/l)    1.11                    1.00
   Reduced chisquare           1.00                    0.99
Analysis method tested: Simple
   Error limits for Reduced chisquare      >0.11  and  <3.09
   Warning limits for Reduced chisquare    >0.21  and  <2.41

                    -- MC-Precision Option PASSED --
```

ARCHIVES OPTIONS

Archives
List Assay Log
List MC Log
List Measurement Log

The log file archives the measurement results. Currently all measurement results are stored in a single circular file that can contain 500 entries. The three List Log Options allow the user to output the measurement results or a subset of the results.

List Assay Log

An archival file of the most recent 500 measurements is kept on the system disk. When the file is full, the oldest measurement is replaced by the newest measurement. The

List Assay Log (cont.)

contents can be listed on the operator terminal, printed on the line printer, or written to a file in ASCII format.

When this option is selected, the following dialog box is shown:

```
List MC Log
List entries between two dates
List n entries
List all entries
Return to main menu
```

After selecting one of these options, another dialog box will be presented where the operator specifies which output format is desired. The following dialog box will be presented if the operator chooses a date range:

```
List MC Log
Range (dates) From:  53.01.02
                To:  92.12.12
  Output to Screen:  Y
 Output to Printer:  N
    Output to File:  N
         File Name:
```

The user can select from three output devices. Any combination can be selected. Forty-three characters are allowed for File Name of the ASCII file.

Sample Output

Tokai-mura K-Edge Densitometer — Measurement Control Log

Type	Sample ID	Operator	Result (g/l)	E/S	MC	Cycle	Date
MC-P	item	Jim	220.40 +/- 0.90	E	Passed	Average	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	5/5	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	4/5	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	3/5	92.10.02
MC-P	item	Jim	221.00 +/- 1.23	E	Passed	2/5	92.10.02
MC-P	item	Jim	220.22 +/- 1.23	E	Passed	1/5	92.10.02
MC-B	Ta_7_7	Wilber	123.45 +/- 12.34	S	Failed	1/1	92.09.30
ST	Straight-Thr	Hooter			Passed	1/1	92.09.09
B	Background	Hooter			??	1/1	92.09.09
MC-P	test	Wilber	123.45 +/- 12.34	S	Failed	Average	92.09.01
MC-P	test	Wilber	123.45 +/- 12.34	S	Failed	121/121	92.09.01

The measurement type of Assay is indicated in the first column. The result printed in the fourth column is from either the simple method or the extrapolated method. The selected method is listed in the fifth column under the E/S heading. E indicates the extrapolated-method result was selected.

List MC Log

This option is similar to the List Assay Log Option, but lists only measurement control measurement types: MC–Bias, MC–Precision, Background, and Straight-Through measurements.

When this option is selected, the following dialog box is shown:

List MC Log
List entries between two dates
List n entries
List all entries
Return to main menu

After selecting one of these choices, a dialog box will be presented so the operator can choose the output formats.

List MC Log (cont.)

List MC Log
Range (dates) From: 53.01.02
To: 92.12.12
Output to Screen: Y
Output to Printer: N
Output to File: N
File Name:

The user can select from three output devices. Any combination can be selected. Forty-three characters are allowed for File Name of the ASCII file.

Sample Output

Tokai-mura K-Edge Densitometer Measurement Log

Type	Sample ID	Operator	Result (g/l)	E/S	Quality	Cycle	Date
MC-P	item	Jim	220.40 +/- 0.90	E	Passed	Average	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	5/5	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	4/5	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	3/5	92.10.02
MC-P	item	Jim	221.00 +/- 1.23	E	Passed	2/5	92.10.02
MC-P	item	Jim	220.22 +/- 1.23	E	Passed	1/5	92.10.02
A	123456789012	Jim	220.40 +/- 0.90	E	Passed	Average	92.10.01
A	123456789012	Jim	220.00 +/- 1.23	E	Passed	3/2	92.10.01
A	123456789012	Jim	221.00 +/- 1.23	E	Passed	2/2	92.10.01
A	123456789012	Jim	220.22 +/- 1.23	E	Passed	1/2	92.10.01
MC-B	Ta_7_7	Wilber	123.45 +/- 12.34	S	Failed	1/1	92.09.30
ST	Straight-Thr	Hooter			Passed	1/1	92.09.09
B	Background	Hooter			??	1/1	92.09.09
C	std 001 002	NISHIDA	6.0000 +/- 0.001	E	Passed	2/5	92.09.08
C	std 001 002	NISHIDA	6.0000 +/- 0.001	E	Passed	1/5	92.09.08
MC-P	test	Wilber	123.45 +/- 12.34	S	Failed	Average	92.09.01
MC-P	test	Wilber	123.45 +/- 12.34	S	Failed	121/121	92.09.01

List Measurement Log

This option will allow the user to review all six of the measurement types in sequential order. When this option is selected, the following dialog box is shown:

List Measurement Log (cont.)

List MC Log
List entries between two dates
List n entries
List all entries
Return to main menu

After the operator selects one of these options, a dialog box will be presented.

List MC Log	
Range (dates) From:	53.01.02
To:	92.12.12
Output to Screen:	Y
Output to Printer:	N
Output to File:	N
File Name:	

The user can select from three output devices. Any combination can be selected. Forty-three characters are allowed for File Name of the ASCII file.

Sample Output

Tokai-mura K-Edge Densitometer Measurement Log

Type	Sample ID	Operator	Result (g/l)	E/S	Quality	Cycle	Date
MC-P	item	Jim	220.40 +/- 0.90	E	Passed	Average	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	5/5	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	4/5	92.10.02
MC-P	item	Jim	220.00 +/- 1.23	E	Passed	3/5	92.10.02
MC-P	item	Jim	221.00 +/- 1.23	E	Passed	2/5	92.10.02
MC-P	item	Jim	220.22 +/- 1.23	E	Passed	1/5	92.10.02
A	123456789012	Jim	220.40 +/- 0.90	E	Passed	Average	92.10.01
A	123456789012	Jim	220.00 +/- 1.23	E	Passed	3/2	92.10.01
A	123456789012	Jim	221.00 +/- 1.23	E	Passed	2/2	92.10.01
A	123456789012	Jim	220.22 +/- 1.23	E	Passed	1/2	92.10.01
MC-B	Ta_7_7	Wilber	123.45 +/- 12.34	S	Failed	1/1	92.09.30
ST	Straight-Thr	Hooter			Passed	1/1	92.09.09
B	Background	Hooter			??	1/1	92.09.09
C	std 001 002	NISHIDA	6.0000 +/- 0.001	E	Passed	2/5	92.09.08
C	std 001 002	NISHIDA	6.0000 +/- 0.001	E	Passed	1/5	92.09.08
MC-P	test	Wilber	123.45 +/- 12.34	S	Failed	Average	92.09.01
MC-P	test	Wilber	123.45 +/- 12.34	S	Failed	121/121	92.09.01

PARAMETERS OPTIONS

User adjustable parameters are accessed with the parameters option. The short menu allows access to two subsets of parameters. See Chapter 4, Parameters Options, for information on complete access.

Parameters
Miscellaneous
Count Times

Miscellaneous Constants

This option allows the user to change some parameters without a password. These changes are stored in the parameter file. When this option is selected, the following dialog box is shown:

Miscellaneous Constants

Instrument Title:	Tokai-mura K-edge Densitometer		
Default Print Level:	Normal		
Lines per page:	58		
Write Spectral Data to Disk:	N		
Directory 1:	c:\tokai		
Directory 2:			
Directory 3:			
Directory 4:			
Automatic Background:	None	Hour:	22:00
Automatic Straight-Through:	Weekly	Hour:	23:59

Instrument Title. This allows the operator to change the title displayed on the top line of the video terminal display while the software is in use.

Print Level. The printout level can be normal, medium, and long. Any warning or error messages from the diagnostics are printed for all printout levels.

Normal - The normal-level printout consists of a header section and a results section, followed by any diagnostic messages. This will be the most frequently used output.

Medium - The medium-level printout includes the net peak areas in addition to the normal output.

Long - The long-level printout includes the medium printout. In addition, information from all of the diagnostic tests is printed.

Debug - The debug-print level includes channel by channel output from the regions used to determine the net peak areas.

Lines per page. This parameter controls the number of lines per line-printer page. We recommend 58 for a laser writer and 64 for a dot matrix printer.

Write Spectral Data to Disk. If this value is changed to *No*, no spectral data will be written during any measurement. This is the recommended choice. If this value is

Write Spectral Data to Disk (cont.)
changed to *Yes*, the directories specified in the next four lines will be used. There will be a maximum of four copies of each spectral file written to different disk\directory choices. A blank in any row will indicate fewer copies. Please note that writing data to diskette is not a fast process. One file can be written during the measurements, and the multiple copies can be generated after all measurements are complete. Only the first disk\directory is checked for previous use of the filename. If a match is found, the run number is incremented to avoid overwriting the first file.

Automatic Background. TBD

Automatic Straight-Through. TBD

Count Times

If this option is selected, the following dialog box is presented. Use the arrow keys to move to the entry of interest, then type the new count time desired.

Count Times in Seconds

Measurement Type	Number of Measurements	No Source	Co-57	Se-75
Assay	2		500	500
Background	1	300		
Straight-Through	1		2000	2000
MC-Bias	1		300	300
MC-Precision	15		500	500
Calibrate	10		100	100

The number of measurements and the measurement types are listed for information purposes. Neither can be changed in this option.

MENU/EXIT OPTIONS

These options allow the user to switch between the long and short menus or to exit the KED program.

MENU/EXIT OPTIONS
(cont.)

Menu/Exit
Go to Full Menu Exit

Go to Full Menu

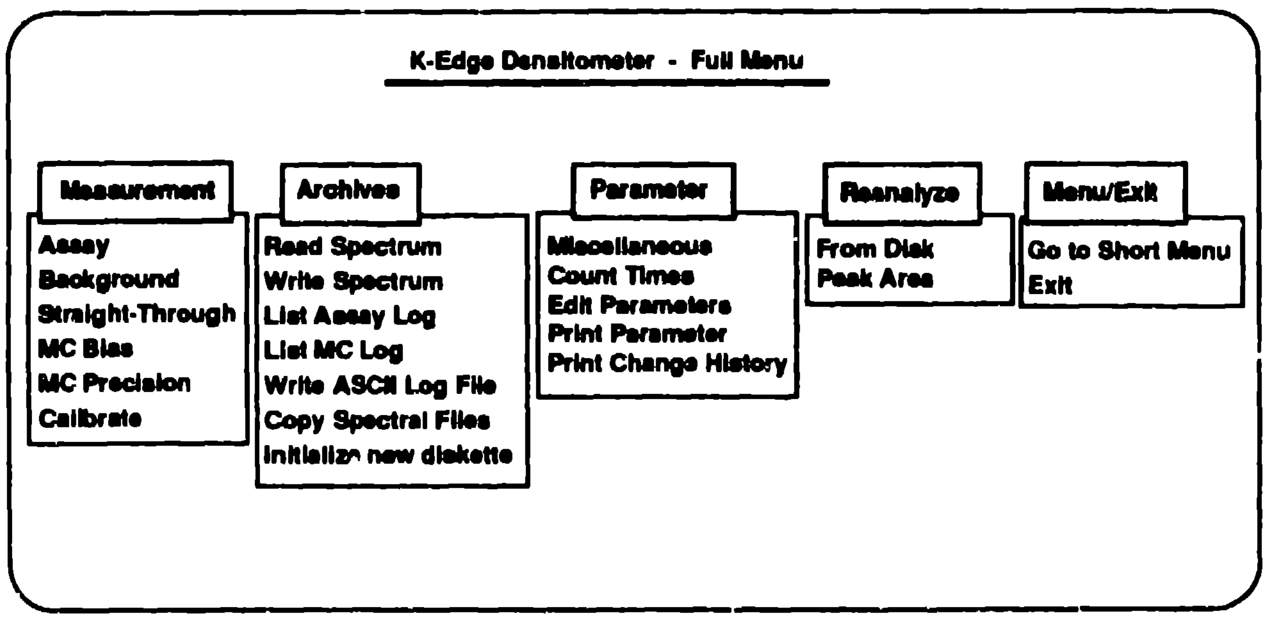
The KED software has two menus: the short menu and the full menu. To go from the short to the full menu requires selecting this option under the MENU/EXIT heading. Approved operator identification is required for this option to be exercised (Level 1 privilege). When the KED is in the full menu, this option becomes Go to Short Menu; no password is required to go from the full to the short menu.

Exit

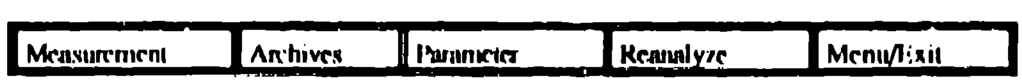
To exit the KED software, use the EXIT Option. Approved operator identification is required for this (Level 1 privilege).

USING THE FULL MENU

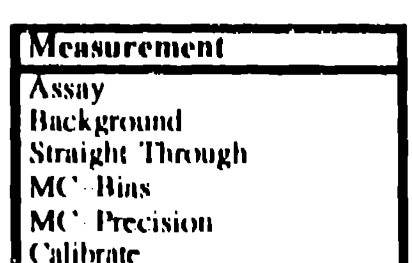
In this chapter you will learn about the options in the full menu. The parameter menu will be discussed in the next chapter.



In the full menu, there are five object headings. *Analysis* is a new heading not found in the short menu. Only options not discussed in the short menu will be discussed here, except that the options under the parameter heading will be discussed in Chap. 4.



MEASUREMENT OPTIONS



MEASUREMENT OPTIONS (cont.)

There are six options in the measurement heading, one more than in the short menu: calibrate.

Calibrate

The Calibration Option is similar to an MC–Precision Option. Repeated measurements are performed on a calibration solution, and the average result (both calibration constants) is printed out at the end of the option. Statistical tests are made on the measurement set.

Operator Entries. In addition to the usual entries, the operator is required to enter the plutonium concentration in grams per liter. If the uncertainty in the concentration is entered for the sigma (sample concentration), the result will include that in the error estimation.

Calibrate Information	
Operator:	
Sample ID:	
Sample Concentration (g/l):	
sigma(g/l):	
Remarks:	

Count Times and Number of Cycles. We recommend counting long enough so that the uncertainty in the calibration constant is about four times less than the uncertainty in a typical assay, up to 0.1%. The count time can be changed in the PARAMETER Count Time Option, the number of cycles can be set in the PARAMETER Edit Parameter Option under calibration constants.

Output. The short output of the Calibrate Option only includes a summary. The reduced chi square test ca· help to determine if the variation in the measurements is because of counting statistics or if it has additional systematic effects.

The medium output of the Calibrate Option adds a printout from each cycle. This printout will include the normalized net peak areas. The long output also prints the diagnostic tests for each cycle. The debug printout has additional

Output (cont.)
information and was useful as the program was being written and for the initial testing.

Sample Summary Printout.

```
                                                    Measurement Type: CALIBRATE
Sample ID: Pufoil#1                                 Measurement Date: 92.11.05
Operator: Jim                                                       Cycle: 5

Remarks: testing tighter FWHM limits
Straight-Through Date: 92.11.03                 Constants File Date: 92.11.05
Live time (Se-75) = 300s                            Live time (Co-57) = 300s

                                 Calibration Summary

Analysis Method tested: Simple

Number of Measurements: 5

                                   Simple              Extrapolated
                                --------------         ------------
Average Result (cc/g):             6.0000                 6.1000
Standard Deviation (cc/g):         0.0610                 0.0600
Reduced Chisquare:                 1.67                   1.66
```

ARCHIVES OPTIONS

Read Spectrum

This option can be used to recall a spectrum from disk and place it into the S100-board memory. The file format is the format specified by Canberra for the S100. This function is also available under the S100 software. It is of little use unless the user can look at the spectrum. The operator must specify the complete file name including the disk unit. See the section on Spectral Display for directions to observe the spectra.

Write Spectrum

This option can be used to write a spectrum from the S100 memory to the disk. The file format is the format specified by Canberra for the S100. This function is also available under the S100 software. The user can use the S100 software to look at the spectra later. The operator must specify the complete file name including disk unit.

REANALYZE OPTIONS

REANALYZE
From Disk
Peak Areas

The REANALYZE menu contains options to repeat the analysis of recorded spectra.

From Disk

When this option is selected, the following dialog box is shown:

Analysis from Disk	
Operator:	
Sample ID:	
Sample Spectral Files	
Se-75:	
Co-57:	
REMARKS:	

This option requires the operator to supply the sample file names. The software will search for these files. If the files are not found, the software will indicate which ones need to be entered correctly. We recommend that the operator use the REMARKS to specify why the analysis from disk is being done.

The printout of this option is similar to the regular assay; the names of the files on which the analysis is based are included.

Peak Areas

This option allows the operator to determine the peak areas in a single spectrum stored on disk. When this option is requested, the following dialog box will be shown:

Analyze Peak Areas	
Spectrum file name:	c:\
Which source:	Blank
Vary FWHM coefficients:	N

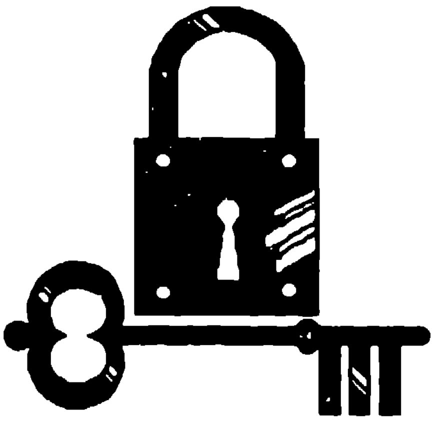
In this option, the program will use the spectrum stored in the memory of the S100 if the entry for the spectrum file name is empty. The operator can select the blank, ^{75}Se, or ^{57}Co source peak information and fitting regions with which to analyze the spectrum. The "vary FWHM coefficients" is not used for the summation method of determining the net peak area. If peak fitting is selected for determining the net peak area, then the operator can control whether to vary the FWHM coefficients. The FWHM parameters may all be allowed to vary, or only the first term may be allowed to vary, or all FWHM parameters may be fixed. See the Appendix for a discussion of the FWHM parameter definitions.

GENERAL

In this chapter you will learn these things about the parameter menu:

- How to edit parameters
- How to print parameters, and
- How to print the history of parameter changes.

The parameter file is the key to the KED system.



Parameters
Miscellaneous
Count Times
Edit Parameters
Print Parameters
List Change History

The Miscellaneous and Count Times Options have been discussed in Chap. 2 as part of the short menu. The other three options are discussed below.

EDIT PARAMETERS

This is the option used to modify the parameters used in the KED analysis and software. When this option is selected, the following dialog box is shown:

EDIT PARAMETERS
(cont.)

Edit Which Parameters?
Peak Information
Peak Fitting Regions
Peak Fitting Constants
FWHM & Centroids
Stabilizer Settings
Calibration Constants
Assay Test Criterion
Measurement Control
Operator Passwords
Return to Main Menu

The first two options use a more general format than the other options. They require different values for each transmission source configuration. Three types of transmission source configurations exist:

1. Background or no source,
2. ^{75}Se source, and
3. ^{57}Co source.

The information in these two options must be consistent. The code assumes that the region number is consistent between the two options. The other options are independent of the transmission source.

Moving Between Cells

Both the Peak Information Option and the Peak Fitting Regions Option list the parameters in spread-sheet form. Use the up and down arrows to change between rows. Use the tab and left arrow keys to change between cells. To edit all other parameters, the cursor is moved between entries by the up and down arrow keys.

Change History

After the operator edits parameters, the program will ask the operator to enter a comment. The user might indicate which parameters were changed. These comments can be reviewed in the List Change History Option.

Peak Information

The peak fitting constants depend on which transmission source in the Geneva mechanism is being used. Different peak fitting parameters are allowed to vary for the analysis of each source. When the Peak Information Option is selected, the following dialog box wi!l be shown:

Edit Peak Information for:
Blank source
Se-75 source
Co-57 source
Return to Edit Menu

The user selects the type of spectra corresponding to the parameters to be edited and presses enter. The following dialog box is shown when the ^{57}Co source is selected:

Peak Information (Co-57 Source)

Pk No	Isotope Name	Peak Energy	Branching Ratio	Area Fixed To Pk	Area Summed With Pk	Used For Energy	Used For FWHM	Used For Shape
1	Cd-109	88.036	0.000E+000	0	0	Y	Y	N
2	Co-57	122.060	0.000E+000	0	0	Y	Y	N
3	Co-57	136.471	0.000E+000	0	0	Y	N	N

Notation in the Peak Information Dialog Box. Several features of the peak fitting software are not necessary for the KED and are not implemented in this software version. Additional information is in Appendix A: Peak Fitting.

Area Fixed to Pk. *Not used in KED.*

Area Summed with Pk. *Not used in KED.*

Used for Energy. These peaks are used for the energy calibration.

Used for FWHM. These peaks are used for the Full Width Half Maximum calibration.

Used for Shape. These peaks are used for the peak shape calibration if the appropriate parameter is set under the Peak Fitting Constants Option.

Notation in the Peak Information Dialog Box (cont.)

The Used for Energy and Used for FWHM features yield the values required for the diagnostic tests. See the FWHM & Centroids (Diagnostic Peaks) Option.

If peak fitting is being used (see the Miscellaneous Parameters Option), the Used for Energy, FWHM, or Shape parameters defer to the Energy, FWHM, or Shape parameters FREE settings in the Peak Fitting Constants Option.

Adding or Deleting Peaks. Peaks are added by typing at the end of the table; when the F10 key is pushed to accept all entries, the program will arrange the peaks in order of ascending energy. Peaks can be deleted by typing zero (0.0) for the peak energy. It is important that the information in this option be consistent with the Peak Fitting Regions Option.

Peak Fitting Regions

The region of interest constants depend on which transmission source in the Geneva mechanism is being used. Different peak fitting regions are required for each source. See the Appendix A: Peak Fitting for more information. When the Peak Fitting Regions Option is selected, the following dialog box will be shown:

Edit Peak Fitting Regions for:
Blank source
Se-75 source
Co-57 source
Return to Edit Menu

The user selects the type of spectra corresponding to the parameters to be edited and presses enter. The following dialog box appears when the ^{75}Se source is selected:

Peak Fitting Regions (cont.)

Fitting Region Information (^{75}Se source)

Region Number	[Fitting Range] Low E	High E	[Background #1	#2	#3	#4]	Bkgd Channels	Bkgd Terms
1	86.9	89.3	86.3	86.3	89.4	89.4	5	5
2	119.7	123.7	119.0	119.0	124.	124.	5	5
3	134.0	138.0	133.5	133.5	136.5	138.5	5	5
4	277.0	282.0	276.5	276.5	282.5	282.5	5	5

The parameters are explained in the Appendix. They are

- The boundaries of the peak region for each gamma ray,
- The positions of the background regions around each gamma ray,
- The number of points in each background region, and
- The type of background function used to fit the continuum under the gamma ray peak.

Notation Used in the Peak Fitting Regions Dialog Box. All region data are stored in the parameter file in energy units so that they are independent of the system energy calibration. One must enter all four background regions, but they need not be unique or independent. For example the same background region may be entered twice or two background regions can overlap. If they overlap, the duplicated points are used only once in the background fitting. If two identical regions are entered, only one set of points is used in the fitting, that is, they are not double weighted. The number of points per background region is the same for each region. The actual number used in the fitting in any given area of the spectrum can be adjusted by overlapping the regions or placing two regions adjacent to each other.

The types of background functions are related to the TERMS parameter as follows.

Notation Used in the Peak Fitting Regions Dialog Box (cont.)

TERMS	Type of Bkg Function
1	Horizontal (zero slope) straight line
2	Straight line with slope and intercept
3	Sloping straight line with step function
4	Parabola with step function
5	Step function with zero slope

Regions are analyzed in the order they are listed.

Adding or Deleting Regions. Regions can be added at the end of the table; when the F10 key is pushed to accept all the entries, the program will arrange the regions in ascending order by energies. Regions can be deleted by zeroing the low energy. It is important that the information in this option be consistent with the information in the Peak Information Option.

Moving Between Cells. Use the up and down arrows to change between rows. Use the tab and left arrow keys to change between cells.

Please note that the peak fitting is disabled in this application.

Peak Fitting Constants

This option allows the operator to change the peak-shape-fitting constants used in the analysis. Detailed description of the peak-shape constants can be found in Appendix A. The printout for the Fitting Constants Option is shown below:

Peak Fitting Constants (cont.)

Peak Fitting Constants	
Peak Fit:	N
Energy Calibration Constants	
Gain (KeV/channel):	0.075
Offset (KeV):	-0.0426
Energy Parameters FREE:	Y
FWHM Calibration Constants	
FWHM2 = A1 + A2*E**	
A1 =	12.12345
A2 =	0.025
FWHM Parameters FREE:	Y
Tailing Constants	
Tail = T{exp(T1 + T2*E + (T3 + T4*E)*δch)}*rolloff	
T1 (tailing amplitude):	-.208425
T2 (tailing amp.(energy)):	0.0010728
T3 (tailing slope):	0.2^477
T4 (tailing slope (energy)):	-0.4
Tailing Parameters FREE:	N
Number of Iterations:	2

In the KED program, the peak shape determination should be performed during the ^{75}Se portion of the straight-through run. *Please note that the units are inconsistent in this application. The units for the FWHM constants are channels, not energy in keV.* If any of these parameters are set FREE, then each of the spectrum types under the Peak Information Option must specify which peaks are used for the parameter fit. The initial determination of these parameters is not a trivial exercise. The Peak Area Option in the REANALYSIS menu may or may not be useful for those who attempt this exercise. *Please note that the peak fitting is disabled in this application.*

Peak Fit. This parameter indicates whether peak fitting or simple summation is used to generate the net peak areas. All of the gamma rays in this application are well resolved. Peak fitting will yield lower quality results than the

Peak Fit (cont.)
summation method. The measurement precision will be smaller for the summation method. In addition, the setup and maintenance of the peak fitting parameters is not easy. We recommend setting this parameter to *No*. ***Please note that the peak fitting is disabled in this application. No is the only possible response.***

Number of Iterations in Fit. If peak fitting is used, the number of iterations can be restricted. The iteration involves adjusting the background under the peak(s) by looking at the residual from the fit, then repeating the fitting process. Other applications have suggested that no benefits are found after two or three iterations.

FWHM & Centroids

In each spectrum, specified peaks are checked for resolution, position, and intensity. These diagnostic checks are specified with this option. A printout of the diagnostic peak dialog box is shown below:

FWHM & Centroids (Diagnostic Peaks)

Transmission Source	Peak Energy	Centroid (Channel +/-	Limit Tolerance)	FWHM limit (Channels)	Desired Precision (%)
Blank	88.036	1157.1	2.0	9.4	0.5
Se-75	88.036	1157.1	3.0	9.4	0.2
Se-75	121.110	1629.8	2.0	9.9	0.2
Se-75	136.000	1842.5	3.0	10.1	0.2
Co-57	88.036	1157.1	2.0	9.4	0.2
Co-57	122.060	1644.6	3.0	10.4	0.2

The centroid limit (position) check is a two-sided test because the spectra can drift in either direction. The limits on the peak centroid must be fairly tight when using the region-of-interest summation method to determine the peak areas because in the peak fitting, the program determines the energy calibration for each spectrum. So if the peak centroid has changed by several channels, the resulting peak area would still be correct.

The FWHM (resolution) test is an upper limit. The limits on the FWHM are determined by measuring the FWHM at low-counting rates and multiplying by a factor of 1.3.

FWHM & Centroids (cont.)

The limits on the peak centroid and FWHM are printed in the medium and long printout options.

Operator Passwords

Operator password privileges are divided into two levels.

Level 1. The first level allows the operator to change between the full menu (requires the operator's name) and the short menu (no restriction).

Level 2. The second level allows the operator to select the Edit Parameter Option. With level two privilege, one can change the calibration constants, as well as the passwords that control access to the calibration constants. The Level 2 capability allows the facility to limit access to critical features of the KED software.

Stabilizer Settings

The controls of the stabilizer are set with this option. Note that each transmission source condition requires different gain-stabilizer parameters. The stabilizer manual describes the parameters.

Stabilizer Settings

	Background	Se-75	Co-57
Gain			
Peak Channel:	3893	3893	1857
Window Width:	11	17	11
Range:	0.500	0.500	0.500
State:	Off	On	On
Zero			
Peak Channel:	1157	1157	1157
Window Width:	11	11	11
Range:	0.500	0.500	0.500
State:	On	On	On

Port: 1 Baud Rate: 9600 Parity: None

Calibration Constants

In this option, the calibration constants can be changed. The calibration constant dialog box is shown below.

Calibration Constants

Simple Method:	6.1234	±	.0012
Extrapolation Method:	6.4321	±	.0021
Calibration Date:	92.11.30		
Number of measurements per standard:	10		

The number of measurements per standard is chosen from a list that appears when the F2 button is pressed. The replicate measurements are checked for consistency.

Assay Test Criterion

The Aaron bubble test for each assay has two parameters as explained in the appendix. The dialog box is shown below.

Assay Test Criterion

Two Measurement Test (sigma):	3.18
Three Measurement Test (sigma):	1.95
Analysis method to test:	Simple

Please note that the user must select which result is tested. We recommend that the simple result be used.

Measurement Control

When the measurement control parameters are selected from the edit menu, a choice must be made with the following dialog box:

Edit Measurement Control for:
Background & Straight-Through
Bias & Precision
Return to Edit Menu

Measurement Control - Background & Straight-Through

For both of these measurement types, there is a maximum time allowed before the measurement type must be repeated successfully. When this time is exceeded and the check has not been performed, an assay will not be permitted. If the

Measurement Control - Background & Straight-Through (cont.)

most recent measurement of the type has failed a diagnostic, supervisor action is needed to proceed. An example of the Background & Straight-Through dialog box is shown below.

Measurement Control - Background & Straight-Through

Background:

Days between checks: 90

Date of last check: 92.3.16

	#1	#2	#3	#4
Peak Energy:	121.1	122.1	59.5	129.3
Warning Limit:	0.0005	0.0005	0.0010	0.00005

Straight-Through:

Days between checks: 7

Date of last check: 92.3.16

	Se-75	Co-57	Cd-109
Halflife (days):	118.452	271.651	464.00
Precision of check (%):	0.50	0.50	0.50

Four peak regions, specified by energy, can be checked in the background spectra. If the normalized counts exceed the specified value, a warning is printed.

The program compares each background or straight-through measurement with the preceding measurement of the same type. If the change in gamma-ray intensity is not consistent with the predicted half-life decay, the operator is warned.

MC Bias & Precision

For each of these measurement types, there is a maximum time allowed before the measurement type must be repeated successfully. When this time is exceeded and the check has not been performed, an assay will not be permitted. If the most recent measurement of one of these types failed the diagnostic tests, then supervisory action is required to

MC Bias & Precision (cont.)

perform an assay. An example of the measurement control dialog box is shown below.

Measurement Control - Bias & Precision
Bias:
Days between checks: 90
Date of last check: 92.3.16

	#1	#2	#3	#4	#5
Bias sample identification:	Ta0/7	Ta7/15	Ta_7_7	Pu01	Pu02
Standard Value:	220.12	240.12	0.00	201.12	0.00
Historical standard deviation:	2.00	2.00	2.00	2.00	0.00

Precision:
Days between checks: 90
Date of last check: 92.3.16
Number of Measurements: 25

The operator may s re up to five different standard identifications and values for the MC–Bias Option. When the MC–Bias Measurement Option is exercised, the sample ID will be chosen from this list.

The number of measurements for an MC-Precision Option can be selected from the list seen when the F2 button is pressed. A larger number of measurements yields a more precise estimate of the standard deviation of the measurements, consequently the test limits are tighter for that case.

PRINT PARAMETERS

This option allows the operator to print the parameters used in the program. The program can either print all the parameters or it can print different parameter groupings. The following dialog box will be shown when this option is selected:

PRINT PARAMETERS (cont.)

Print Which Parameters?
Peak Information
Peak Fitting Regions
Peak Fitting Constants
FWHM & Centroids
Operator Passwords
Stabilizer Settings
Calibration Constants
Assay Test Criterion
Measurement Control
Count Times
Miscellaneous Constants
All of them
Return to the Main Menu

The operation of these options is similar to the Edit Parameter Options, except that the output will be printed instead of allowing the operator to change the parameters.

All of Them

This option allows the operator to print all the parameters used in the KED program, *except for the operator passwords*. The user may also choose to print a subset of the parameter file.

KED Parameter File 13-May-92 16:11

Peak Information (Background)

Pk No	Isotope Name	Peak Energy	Branching Ratio	Area Fixed To Pk	Area Summed With Pk	Used For Energy	Used For FWHM	Used For Shape
1	Am-241	59.595	0.000E+000	0	0	N	N	N
2	Cd-109	88.036	0.000E+000	0	0	Y	N	N
3	Se-75	121.115	0.000E+000	0	0	N	N	N
4	Co-57	122.060	0.000E+000	0	0	N	N	N
5	Pu-239	129.290	0.000E+000	0	0	N	N	N
6	Co-57	136.471	0.000E+000	0	0	N	N	N
7	Se-75	279.528	0.000E+000	0	0	N	N	N

All of Them
(cont.)

Peak Information (Se-75 Source)

Pk No	Isotope Name	Peak Energy	Branching Ratio	Area Fixed To Pk	Area Summed With Pk	Used For Energy	Used For FWHM	Used For Shape
1	Cd-109	88.036	0.000E+000	0	0	Y	Y	N
2	Se-75	121.115	0.000E+000	0	0	Y	Y	N
3	Se-75	136.000	0.000E+000	0	0	Y	Y	N
4	Se-75	279.528	0.000E+000	0	0	Y	N	N

Peak Information (Co-57 Source)

Pk No	Isotope Name	Peak Energy	Branching Ratio	Area Fixed To Pk	Area Summed With Pk	Used For Energy	Used For FWHM	Used For Shape
1	Cd-109	88.036	0.000E+000	0	0	Y	Y	N
2	Co-57	122.060	0.000E+000	0	0	Y	Y	N
3	Co-57	136.471	0.000E+000	0	0	Y	N	N

Fitting Region Information (Background)

Region Number	[Fitting Range] Low E	High E	[Background #1	#2	#3	#4]	Bkgd Channels	Bkgd Terms
1	57.5	61.5	57.0	57.0	62.0	62.0	5	5
2	86.9	89.3	86.3	86.3	89.4	89.4	5	5
3	119.7	123.7	119.0	119.0	124.0	124.0	5	5
4	128.1	130.4	127.6	127.6	130.5	130.5	5	5
5	134.0	138.0	133.5	133.5	138.5	138.5	5	5
6.	277.0	282.0	276.5	276.5	282.5	282.5	5	5

Fitting Region Information (^{75}Se source)

Region Number	[Fitting Range] Low E	High E	[Background #1	#2	#3	#4]	Bkgd Channels	Bkgd Terms
1	86.9	89.3	86.3	86.3	89.4	89.4	5	5
2	119.7	123.7	119.0	119.0	124.	124.	5	5
3	134.0	138.0	133.5	133.5	138.5	138.5	5	5
4	277.0	282.0	276.5	276.5	282.5	282.5	5	5

Fitting Region Information (^{57}Co source)

Region Number	[Fitting Range] Low E	High E	[Background #1	#2	#3	#4]	Bkgd Channels	Bkgd Terms
1	86.9	89.3	86.3	86.3	89.4	89.4	5	5
2	119.7	123.7	119.0	119.0	124	124	5	5
3	134.0	138.0	133.5	133.5	138.5	138.5	5	5

All of Them
(cont.)

Peak Fitting Constants

Energy Calibration Constants

Gain (KeV/channel): 0.069999 KeV/channel
Offset (KeV): 7.05699 KeV
Energy Parameters Free: Y

FWHM Calibration Constants

FWHM**2 = A1 + A2*E + A3/E

a1: 25.6178 a2: 0.028649 a3: -9976.6563
FWHM Parameters Free: Y

Tailing Constants

T1 (tailing amplitude): -3.90650
T2 (tailing energy): 0.0150908
T3 (tailing slope): 0.34008
T4 (Gaussian Roll-off): -0.40000
Tailing Parameters Free: Y

FWHM & Centroids (Diagnostic Peaks)

Transmission Source	Peak Energy	Centroid Limit (Channel +/- Tolerance)		FWHM limit (Channels)	Desired Precision (%)
Blank	88.036	1157.1	2.0	9.4	0.5
Se-75	88.036	1157.1	3.0	9.4	0.2
Se-75	121.110	1629.8	2.0	9.9	0.2
Se-75	136.000	1842.5	3.0	10.1	0.2
Co-57	88.036	1157.1	2.0	9.4	0.2
Co-57	122.060	1644.6	3.0	10.4	0.2

Stabilizer Settings

	Background	Se-75	Co-57
Gain			
Peak Channel:	3893	3893	1857
Window Width:	11	17	11
Range:	0.500	0.500	0.500
State:	Off	On	On
Zero			
Peak Channel:	1157	1157	1157
Window Width:	11	11	11
Range:	0.500	0.500	0.500
State:	On	On	On

Port: 1 Baud Rate: 300 Parity: None

All of Them
(cont.)

Calibration Constants

Simple Method:	6.1234	±	.0012
Extrapolation Method:	6.4321	±	.0021
Calibration Date:	92.11.30		
Number of measurements per standard:	10		

Assay Test Criterion

Two Measurement Test (sigma):	3.18
Three Measurement Test (sigma):	1.95
Analysis method to test:	Simple

Measurement Control - Background & Straight-Through

Background:
Days between checks: 90
Date of last check: 92.3.16

	# 1	# 2	# 3	# 4
Peak Energy:	121.1	122.1	59.5	129.3
Warning Limit:	0.0005	0.0005	0.0010	0.00005

Straight-Through:
Days between checks: 7
Date of last check: 92.3.16

	Se-75	Co-57	Cd-109
Halflife (days):	118.452	271.651	464.00
Precision of check (%):	0.5	0.5	0.50

Measurement Control - Bias & Precision

Bias:
Days between checks: 90
Date of last check: 92.3.16

	# 1	# 2	# 3	# 4	# 5
Bias sample identification:	Ta0/7	Ta7/15	Taxxx	Pu01	Pu02
Standard Value:	220.12	240.12		201.12	
Historical standard deviation:	2.	2.		2.	
Warning Limit:	2.00				
Error Limit:	4.00				

Precision:
Days between checks: 90
Date of last check: 92.3.16
Number of Measurements: 15

All of Them
(cont.)

Count Times in seconds

Measurement Type	Number of Measurements	No Source	Co-57	Se-75
Assay	2		500	500
Background	1	300		
Straight-Through	1		2000	2000
MC-Bias	1		300	300
MC-Precision	15		500	500
Calibrate	10		100	100

Miscellaneous Constants

Instrument Title:	Tokai-mura K-Edge Densitometer	
Print Level:	Normal	
Write Data to Disk:	N	
Automatic Background:	Daily	Hour: 22:00
Automatic Straight-Through:	Weekly	Hour: 23:59
Peak Fit:	N	
Number of Iterations in Fit:	2	

Write Data to Disk:Directory

LIST CHANGE HISTORY

This option allows the operator to print the history of changes made on the KED system. It keeps a history of the changes made to the parameter file and which measurement control runs are performed on the system.

Each entry lists the date and time and the comment the operator entered. A hard copy can be obtained by adjusting the display and then using the |print screen| button.

GENERAL

To see the MCA spectral display, one must exit the KED software. This can be accomplished in two ways.

Method 1 requires that the user start Windows 3 and the S-100 software before starting the KED software. Then the user can collapse the display to an icon. This releases the S-100 board so that the KED program can attach to it. When at the DOS prompt, the user can start the KED program as normal, collapse the KED program to an icon, and then toggle between KED and the S-100 display icons. Once the Windows package is started, the user can toggle into and out of Windows 3 by typing ctrl-alt. This type of exit to DOS will not detach the S-100 board. If the user then runs KED, eventually the system will stop because of a conflict between the two pieces of software competing for the S-100 board.

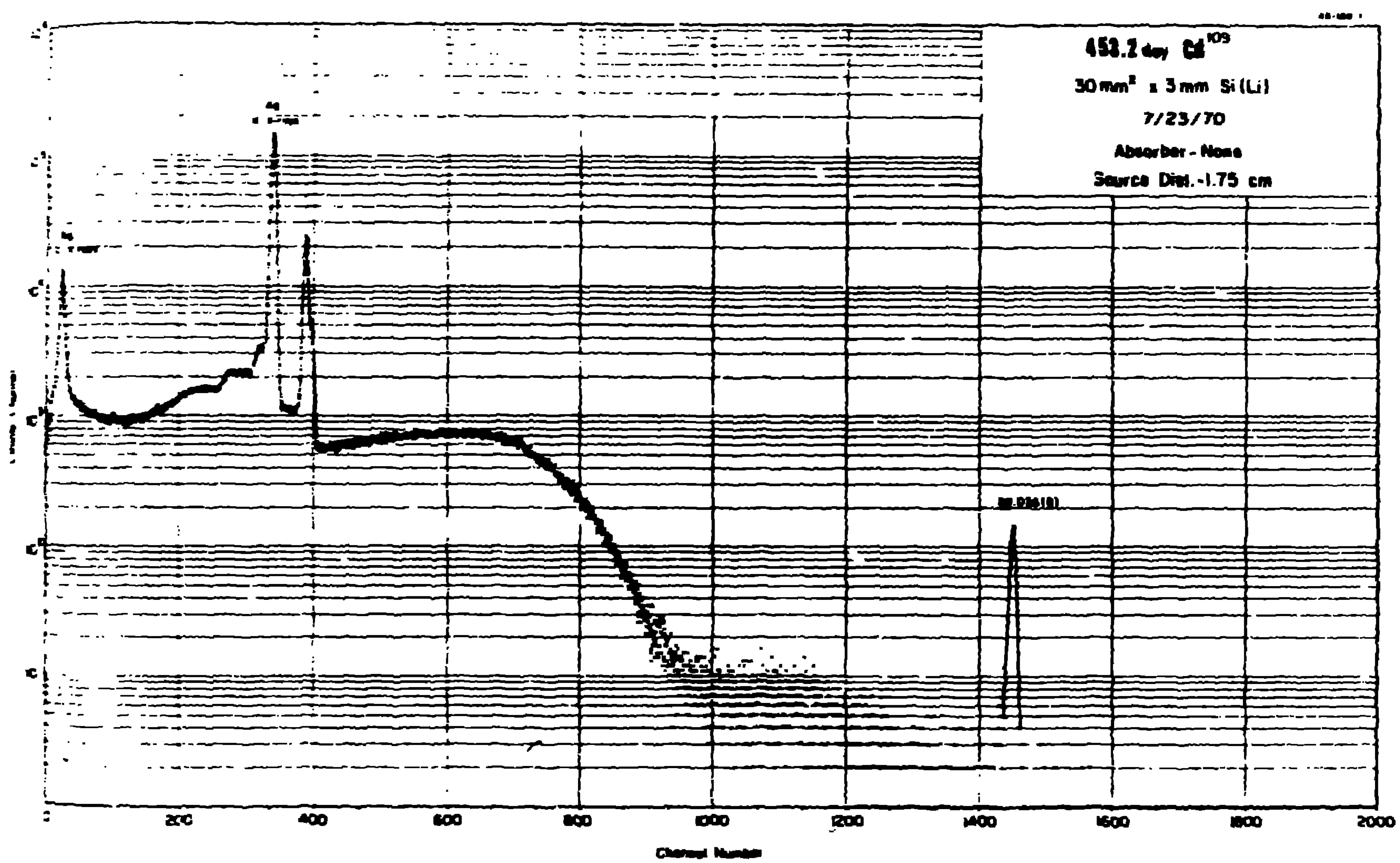
Method 2 requires the user to run either the S-100 software under windows or the KED software. The user performs an EXIT Option of the first program before starting the other one.

In any event, typing "WIN" to a DOS prompt will start Windows 3.0. Then the user activates the S-100 button with the mouse to start the S-100 software.

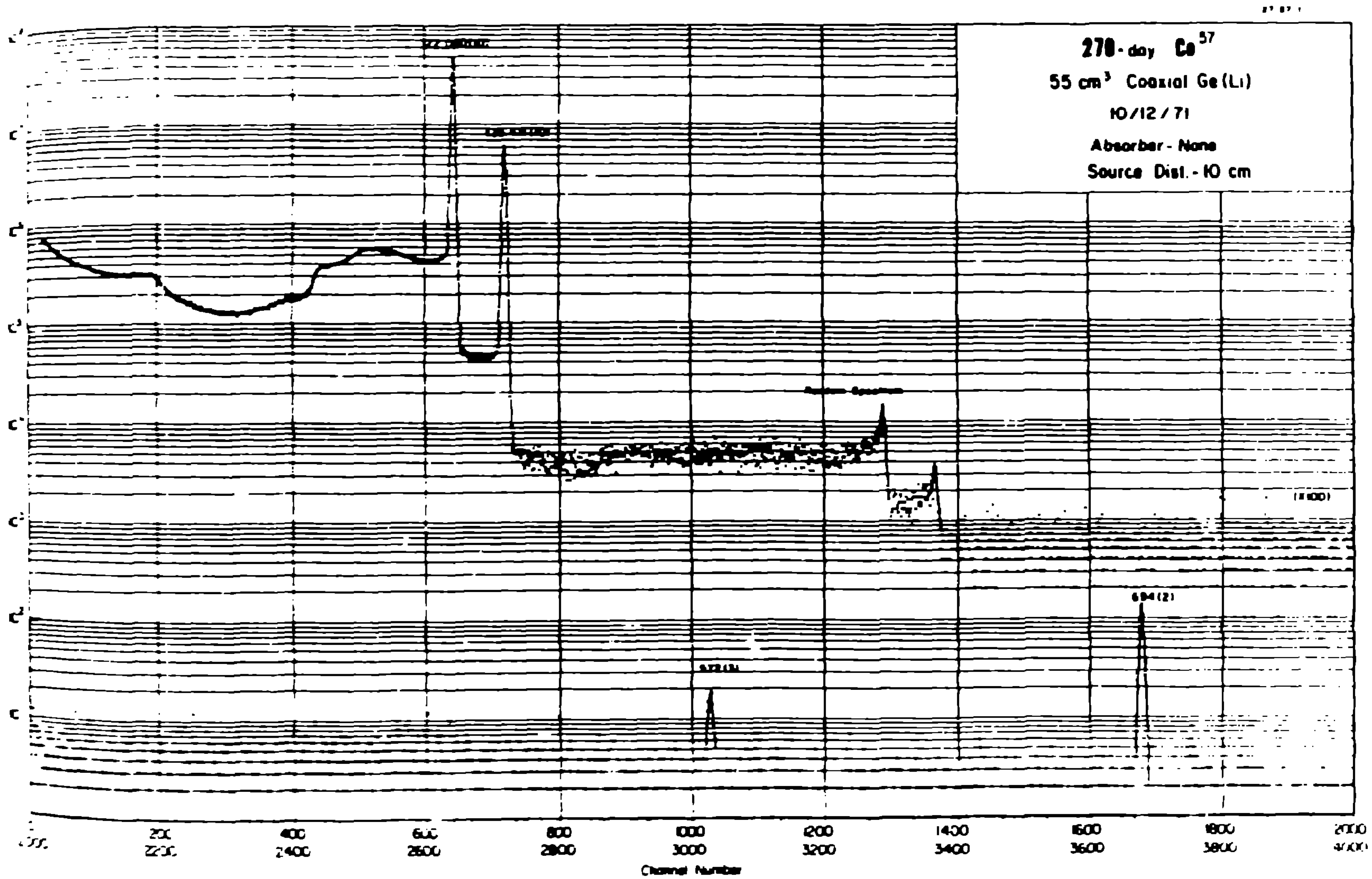
Source Spectra

Spectra from the three radioactive sources are in the next three figures. The ^{109}Cd is the rate-loss source and the 88.036-keV gamma ray is expected to be present in every spectrum. The ^{75}Se and ^{57}Co are the two transmission sources.

Please note that lead shields can fluoresce at 72.8, 74.7, 84.4, and 84.9 keV, while tungsten can fluoresce at 58.0, 59.3, 67.2, and 69.1 keV. Some ^{109}Cd sources are contaminated with ^{113m}Cd, which has a gamma ray at 263.7 keV.

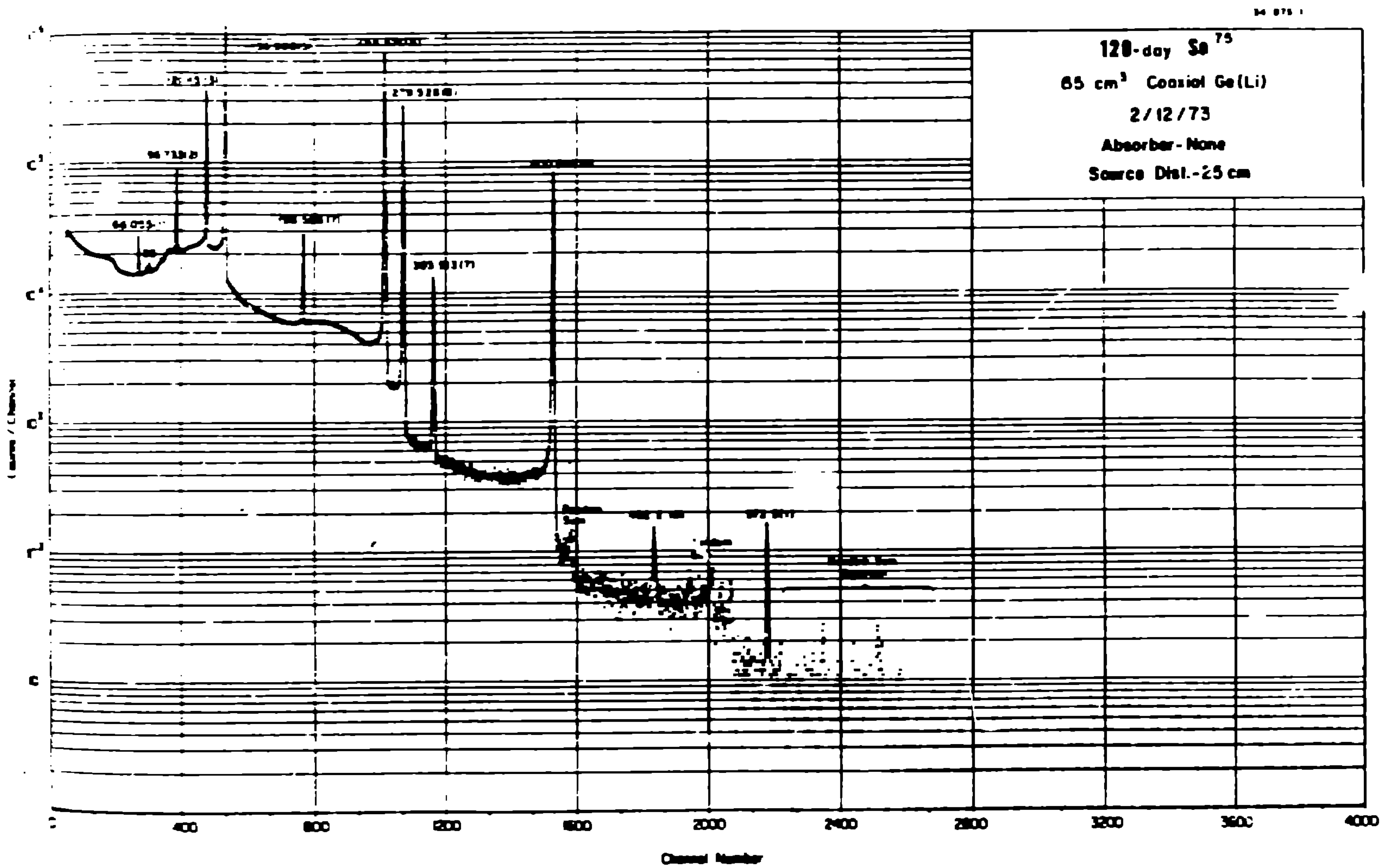


KED SPECTRAL DISPLAY



KED

SPECTRAL DISPLAY



SPECTRAL DISPLAY

KED

GENERAL

In the appendix, you will learn about

- Analysis physics of KED software,
- Amplifier gain and ADC zero adjustment,
- Calibration,
- FEIR determination, and
- Trouble shooting.

ANALYSIS ALGORITHMS OF THE KED SOFTWARE

We recommend the use of the ROI summation method over peak fitting for applications that have gamma-ray peaks that are isolated by energy. The net peak area determination has a smaller uncertainty and it is simpler to implement. The determination of the tail portion of the peak shape parameters is difficult to perform and quite sensitive to which peaks are selected.

Peak Region Summation

The net peak area is determined by subtracting the background from the measured counts, channel-by-channel. The net counts are summed over the region of interest to obtain a result.

Background Determination

Four background regions can be specified. Each region is the same width. Each region is specified by the starting channel. If the user prefers to use two background regions, the first and second regions should be identical and the third and fourth regions should be identical.

A choice between five functions to fit the background continuum is offered by the terms parameter:

Background Determination (cont.)

Terms	Description
0	no background - the background is all zeros
1	flat background - the background is the average of the counts in the first region
2	linear background - the background is a straight line connecting the average counts in the first two regions
3	linear step - the background is a step superimposed on a slope
4	exponential - the background will be an exponential function fit to the two background regions
5	flat step - the background will make a smooth transition from the average of the counts in the first region to the average of the counts in the second region

The choice of background region is more important for the fitting of multiple peaks that overlap. The KED was delivered with terms set to five.

Energy Calibration

Energy calibration is performed for every spectrum. Peak centroids for all peaks in the energy calibration list are needed to carry out the segment-by-segment linear energy calibration. In addition, the centroids of specified peaks are compared to diagnostic limits for each spectrum type. The peak centroids are found by fitting a quadratic in channel number to the net counts. The fitting range is five channels wide, centered on the channel where the default energy calibration predicts the peak will be. The energy calibration is then assumed to be linear between each pair of energy calibration peaks in the list.

FWHM Determination

The FWHM's of specified peaks are compared to diagnostic limits for each spectrum type. The determination of the FWHM is made by fitting a quadratic in channel number to the logarithm of the net counts. The fitting range is from 0.75 • HT on the lower energy side of the centroid to

FWHM Determination (cont.)

0.25 • HT on the higher energy side of the centroid, where HT is the height of the peak shape.

K-EDGE DENSITOMETRY

The net peak areas, resolutions (FWHM), and centroids are calculated from the raw data in the same way for all gamma-ray instruments. These algorithms have been carefully checked and should not be modified without careful consideration and rigorous testing to ensure no possibility of an error. The measured net peak areas from the five different data acquisitions follow some conventions. *B* represents peak area results from the background measurement, A_0 represents results from a straight-through measurement with no sample present, and *A* represents results from an assay, MC, auto cycle, or calibration measurement with a sample. The background measurement is one acquisition with no transmission source (blank), all other measurements are based on two acquisitions with the selenium and cobalt sources. The value in parentheses is the gamma-ray energy associated with the peak area, and the letter indicates which source was in place.

The measured net peak areas from the five different data acquisitions are

from the background:

$B(88)$
$B(121)$
$B(122)$
$B(136)$

from the cobalt source, straight-through (no sample):

$A_0(88,C)$
$A_0(122,C)$

from the selenium source, straight-through (no sample):

$A_0(88,S)$
$A_0(121,S)$
$A_0(136,S)$

from the cobalt source, sample measurement:

$A(88,C)$
$A(122,C)$

from the selenium source, sample measurement:

$A(88,S)$
$A(121,S)$
$A(136,S)$.

K-EDGE DENSITOMETRY (cont.)

Notes: a net peak area corresponding to the 88-keV gamma ray from the ^{109}Cd rate-loss source is obtained in each acquisition and the five different values must not be mixed up. There is a 136-keV gamma ray from both ^{57}Co and ^{75}Se; we use the net peak area from the ^{75}Se.

Two methods are used in this instrument to calculate the plutonium concentration from the measured net peak areas. The simple method was implemented in 1979 in Tokai I. It works quite well, but has a small bias if there are large quantities of other SNM present. For example, 100 g/l of uranium gives the same result as -1.5 g/l of plutonium. The extrapolation method avoids that bias for a small increase in the measurement uncertainty. However, the samples at the Tokai plant are believed to never have significant quantities of high-atomic-number impurities. In the Simple Method, each net peak area is normalized by the corresponding rate-loss-source net peak area:

$$\text{that is } B(122,n) = \frac{B(122)}{B(88)}$$

$$\text{or } A_0(122,C,n) = \frac{A_0(122,C)}{A_0(88,C)}$$

$$\text{or } A(121,S,n) = \frac{A(121,S)}{A(88,S)} \ .$$

No background subtraction is made for the densitometry measurement. Several reasons support this:

(1) The gamma rays used for assay do not come from the sample.

(2) The detector is tightly collimated and well shielded. During an assay, most of the gamma-ray signal comes from the transmission sources through the sample, not from the sample.

(3) No sample is present for the background measurement. Any significant contamination of the sample cell would be detected with the background limit test.

K-EDGE DENSITOMETRY (cont.)

Three transmissions are computed, $T(121)$, $T(122)$, and $T(136)$. Each transmission is computed in the form given explicitly for 121 keV:

$$T(121) = \frac{A(121)}{A_0(121)}$$

$$= \frac{\dfrac{A(121,S)}{A(88,S)}}{\dfrac{A_0(121,S)}{A_0(88,S)}}$$

The relative uncertainty in the transmission at 121 keV is

$$\frac{\sigma^2[T(121)]}{T^2(121)} = \frac{\sigma^2[A(121,S)]}{A^2(121,S)} + \frac{\sigma^2[A(88,S)]}{A^2(88,S)} + \frac{\sigma^2[A_0(121,S)]}{A_0^2(121,S)} + \frac{\sigma^2[A_0(88,S)]}{A_0^2(88,S)}$$

where $\sigma(x)$ is the absolute uncertainty (1 sigma) in x. This can also be written as

$$\sigma_r^2[T(121)] = \sigma_r^2[A(121,S)] + \sigma_r^2[A(88,S)] + \sigma_r^2[A_0(121,S)] + \sigma_r^2[A_0(88,S)] \; ,$$

where $\sigma_r(x) = \dfrac{\sigma(x)}{x}$.

For the special case of an MC Precision measurement, the same straight-through data is used for each result. The straight through data should be treated as a constant in the error estimate. Therefore the following expression is valid.

K-EDGE DENSITOMETRY (cont.)

$$\sigma_r^2[T(121)] = \sigma_r^2[A(121,S)] + \sigma_r^2[A(88,S)] \ .$$

A half-life correction is made to correct for the elapsed time between the straight-through measurement and the assay.

CF (half life) $= \exp(\lambda \bullet et)$ where

λ = the decay constant for the isotope involved

$$= \frac{\ln(2)}{\text{half - life (isotope)}}, \text{ and}$$

et = elapsed time .

The units in this application will be days for half-life and elapsed time. Three are half-lives involved: one for ^{109}Cd, one for ^{75}Se, and one for ^{57}Co. The ^{75}Se transmission values will be corrected by the ratio of the ^{75}Se to ^{109}Cd corrections.

$$CF(T121) = \frac{\exp[\lambda(Se) \bullet et]}{\exp[\lambda(Cd) \bullet et]}$$

$$= \exp\{[\lambda(Se) - \lambda(Cd)] \bullet et\}$$

$$CF(T136) = \frac{\exp[\lambda(Se) \bullet et]}{\exp[\lambda(Cd) \bullet et]}$$

$$CF(T122) = \frac{\exp[\lambda(Co) \bullet et]}{\exp[\lambda(Cd) \bullet et]}$$

$$= \exp\{[\lambda(Co) - \lambda(Cd)] \bullet et\}$$

Therefore the half life corrected values, T', are:

K-EDGE DENSITOMETRY
(cont.)

$$T'(121) = T(121) \cdot CF(T121)$$

and similarly for $T(122)$ and $T(136)$. The relative uncertainty in the transmissions is unchanged by this correction. The absolute uncertainty is

$$\sigma[T'(121)] = \sigma[T(121)] \cdot CF(T121)$$

and similarly for $\sigma[T'(122)]$ and $\sigma[T'(136)]$.

The simple result for the densitometry measurement is calculated from the two transmissions $T'(121)$ and $T'(122)$:

$$R = \frac{T'(122)}{T'(121)}$$

$$\text{concentration} = \frac{-\ln(R)}{k} \quad ,$$

where k is the calibration constant. The relative uncertainty in the simple method result is calculated from the relative uncertainties in the two transmissions:

$$\frac{\sigma^2(R)}{R^2} = \left\{ \frac{\sigma^2[T'(121)]}{T'^2(121)} + \frac{\sigma^2[T'(122)]}{T'^2(122)} \right\}$$

$$\frac{\sigma^2(\text{concentration})}{\text{concentration}^2} = \frac{\sigma^2(R)}{[R\ln(R)]^2} + \frac{\sigma^2(k)}{k^2}$$

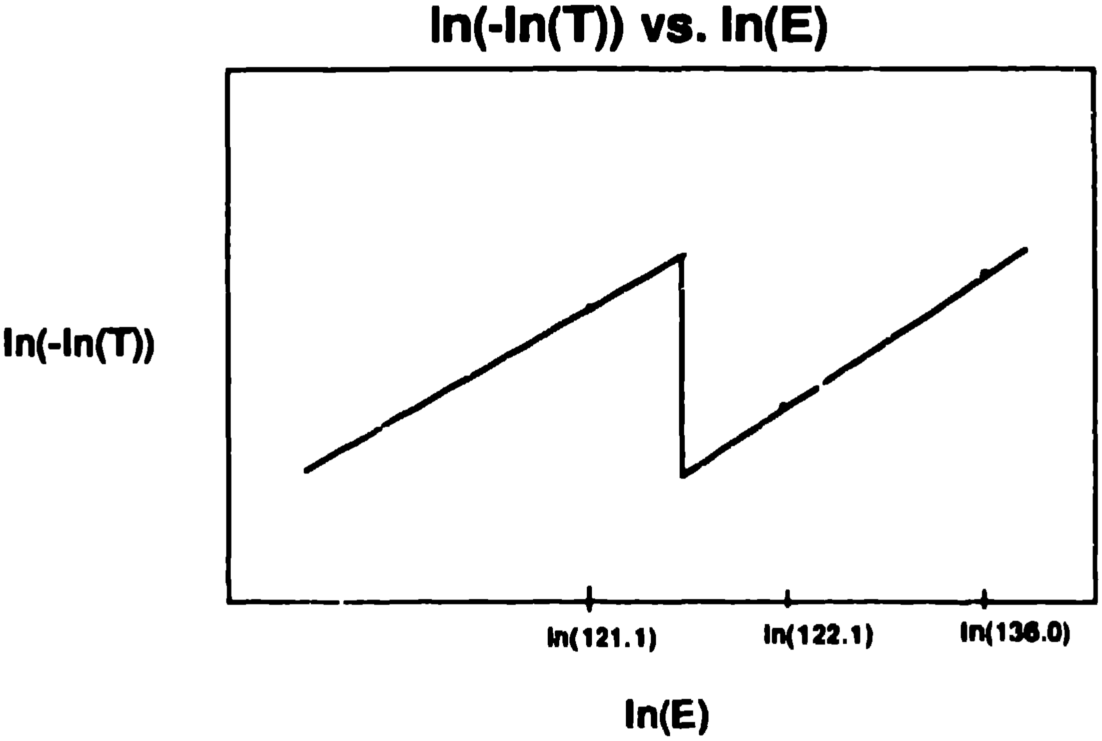
In the calibration option, invert the equation and use the declared concentration:

K-EDGE DENSITOMETRY
(cont.)

$$k = \frac{\ln R}{\text{concentration}}$$

$$\frac{\sigma^2(k)}{k^2} = \frac{\sigma^2(R)}{\{R[\ln(R)]\}^2} + \frac{\sigma^2(\text{concentration})}{\text{concentration}^2} .$$

EXTRAPOLATION TO THE EDGE



In this method, the transmissions above and below the K edge are extrapolated to the edge energy at 121.7 keV. The extrapolation is very nearly linear in ln[-ln(T)] vs ln(E) space. The two transmissions above the edge, $T'(122)$ and $T'(136)$, are used to extrapolate to $T_a(121.7)$, where the a denotes the value above the edge.

$$\ln[-\ln(T_a)] = C \ln[-\ln[T'(122)]] + (1-C) \ln[-\ln[T'(136)]]$$

EXTRAPOLATION TO THE EDGE (cont.)

$$\text{where } C = \frac{\ln(121.795) - \ln(136.00)}{\ln(122.06) - \ln(136.00)}$$

$$= 1.0200978$$

$$\text{and } 1 - C = -0.0200978$$

The formula for the uncertainty in T_a is

$$\sigma_r^2(T_a) =$$

$$\frac{\sigma^2(T_a)}{T_a^2} = \ln^2(T_a)\left\{\frac{C^2\sigma_r^2[T'(122)]}{\ln^2[T'(122)]} + \frac{(1-C)^2\sigma_r^2[T'(136)]}{\ln^2[T'(136)]}\right\}$$

$$\text{where } \sigma_r(x) = \frac{\sigma(x)}{x} .$$

The slope determined above the edge is used below the edge with the transmission determined below the edge, $T'(121)$, to determine $T_b(121.7)$. The slope is actually different, but the bias this assumption introduces is very small.

$$\ln[-\ln(T_b)] = D\left(\ln\{-\ln[T'(122)]\} - \ln\{-\ln[T'(136)]\}\right) + \ln\{-\ln[T'(121)]\}$$

$$\text{where } D = \frac{\ln(121.795) - \ln(121.115)}{\ln(122.06) - \ln(136.00)}$$

$$= -0.05177257$$

The formula for the uncertainty in T_b is

EXTRAPOLATION TO THE EDGE (cont.)

$$\sigma_r^2(T_b) = \frac{\sigma^2(T_b)}{T_b^2} = \ln^2(T_b)\left\{\frac{D^2\sigma_r^2[T'(122)]}{\ln^2[T'(122)]} + \frac{D^2\sigma_r^2}{\ln^2[T'(136)]} + \frac{\sigma_r^2[T'(121)]}{\ln^2[T'(121)]}\right\}$$

The extrapolated result is

$$\text{concentration1} = \frac{-\ln\left[\frac{T_a(121.7)}{T_b(121.7)}\right]}{k1}$$

where $k1$ is the calibration constant. Note that the two calibration constants $k1$ and k are different. We will ignore the small correlation between T_a and T_b that is a consequence of using the same slope; therefore the uncertainty in concentration1 is

$$R1 = \frac{T_a(121.7)}{T_b(121.7)}$$

$$\frac{\sigma^2(R1)}{R1^2} = \frac{\sigma^2[T_a(121.7)]}{T_a^2(121.7)} + \frac{\sigma^2[T_b(121.7)]}{T_b^2(121.7)}$$

$$\frac{\sigma^2(\text{concentration})}{\text{concentration}^2} = \frac{\sigma^2(R1)}{[R1 \cdot \ln(R1)]^2} + \frac{\sigma^2(k1)}{k1^2}$$

In the calibration option use

EXTRAPOLATION TO THE EDGE (cont.)

$$k1 = \frac{-\ln\left[\frac{T_a(121.7)}{T_b(121.7)}\right]}{\text{concentration}1}$$

$$\frac{\sigma^2(k1)}{(k1)^2} = \frac{\sigma^2(R1)}{[R1 \cdot \ln(R1)]^2} + \frac{\sigma^2(\text{concentration})}{\text{concentration}^2}$$

For the special case with no sample, the transmission should be 1.00000. The uncertainty in the counting statistics can cause the transmission to be slightly different from 1.00000. If the transmission is greater than 1.0, then it is not possible to perform ln(-ln(T)), where T = transmission. If any of the three transmission values T121, T122, or T136 exceed 1.0, then we extrapolate in ln(T) vs ln(E) space.

$$-\ln(T_a) = C\{-\ln[T'(122)]\} + (1 - C)\{-\ln[T'(136)]\}$$

where C is defined above. The formula for the uncertainty in T_a is

$$\sigma_r^2(T_a) = C^2\sigma_r^2[T'(122)] + (1 - C)^2\sigma_r^2[T'(136)] .$$

$$-\ln(T_b) = D\{-\ln[T'(122)] + \ln[T'(136)]\} - \ln[T'(121)]$$

where D is defined above. The formula for the uncertainty in T_b is

$$\sigma_r^2(T_b) = D^2\sigma_r^2[T'(122)] + D^2\sigma_r^2[T'(136)] + \sigma_r^2[T'(121)]$$

Tantalum Foil

The use of a tantalum foil in both transmission measurements (121.1 and 122.1 keV) will result in an answer very close to zero. However, placing a tantalum foil into one of the transmission measurements or two foils of different thicknesses into the two transmission measurements will give a nonzero result. This allows a verification of the KED instrument without using plutonium. In fact, if the foil is stable and it is measured precisely, this test of the KED is quite rigorous.

Rate-loss Source Considerations

The 88-keV gamma ray from the ^{109}Cd rate-loss source is analyzed in each spectrum. The 88-keV net peak area is used to normalize all other net peak areas obtained from that spectrum. Consequently, the uncertainty in the 88-keV net peak area affects the uncertainty of every normalized net peak area and subsequently all calculations using the net peak areas. The 88-keV count rate should be greater than 500 counts/s to allow reasonable measurement precision in the K-edge densitometer.

The rate-loss source should be filtered to reduce the low-energy x-rays. Without filtering, these x-rays can contribute to pileup peaks and bias the net peak area determination of the peaks used for the assay. Filters can be chosen so that the count rate in the 88-keV net peak area will be approximately 1000 counts/s and the total count rate will be less than twice the 88-keV count rate. By selecting between copper, brass, tin, and cadmium as a filter material and changing the thickness between 0.5 and 2.0 mm, the user can optimize the 88-keV net peak area and almost eliminate the low energy x-ray peaks.

The ^{109}Cd source and the filters will have to be adjusted annually to preserve adequate measurement precision. A new ^{109}Cd rate-loss source will be required every 4-5 years as the source has a 453-day half-life. To achieve adequate measurement precision, we suggest that a new ^{109}Cd rate-loss source be specified to have 100-200 μCi of activity.

AARON'S BUBBLE TEST FOR ASSAYS

There has been some experience with bubbles in the densitometer samples. Therefore two measurements of each sample are compared. If they agree, the average is accepted. If they do not agree, the sample is mixed and measured a third time. We will assume the measurement uncertainty is the same for all measurements in this comparison. This test was developed by Aaron Goldman and Erwin Kuhn.

first result is X1 ± S1 (from simple method)
second result is X2 ± S2 (from simple method)
average of results is $\underline{x} = (X1 + X2) / 2$
test parameter is $Z1 = (|X1 - X2|) / S1$
if Z1 < 3.18, then average result is accepted
    answer = x ± (S1 / 1.414)
    end of assay !
The final output will contain the following information:
    each measurement result
    the test result
    whether the test passed
    the average result

if Z1 ≥ 3.18, then prompt operator to:
please remove sample,
check sample for bubbles,
place sample into assay position
perform third measurement
third result is X3 ± S3 (from simple method)
average of results is now
    $\underline{x} = (X1 + X2 + X3) / 3$
the value farthest from $\underline{x}$ is x*
test parameter is:
$Z2 = (|\underline{x} - x^*|) / S1$
if Z2 < 1.95 then accept all three answers (note Z1 > 3.18)
    answer = $\underline{x}$ ± (S1 / 1.732)
    end of assay !
The final output will contain the following information:
    each measurement result
    the test result
    whether the test passed
    the average result

if 1.95 < Z2 < 3.18, then reject x*
    answer = $(X_i + X_{i+1}) / 2 \pm (S1 / 1.414)$
    end of assay

The final output will contain the following information:
    each measurement result
    the test result

AARON'S BUBBLE TEST FOR ASSAYS (cont.)

whether the test passed
the average result

if Z2 > 3.18, sample is out of control
must perform DA on this sample

The final output will contain the following information:
each measurement result
the test result
whether the test passed
the average result

Please make the two test values, 3.18 and 1.95, parameters the operator can change in the long parameter change.

MC-PRECISION TESTS

Chi-Square Test

The MC-Precision test requires the acquisition of multiple measurement results. The average and standard deviation of the sample are then computed. The chi-square/degree of freedom, or the reduced chi-square is

$$\chi^2 = \frac{(\text{std dev of sample})^2}{(\text{Est. std dev})^2}$$

The value of the chi-square/degree of freedom is tested against warning limits at 95% confidence and action limits at 99% confidence. These limits are fixed in the software.

Chi-Square Test (cont.)

Number of measurements	degrees of freedom	95% confidence		99% confidence	
	n	$\chi^2_{0.025}$	$\chi^2_{0.975}$	$\chi^2_{0.005}$	$\chi^2_{0.995}$
5	4	0.12	2.79	0.05	3.72
6	5	0.17	2.57	0.08	3.35
7	6	0.21	2.41	0.11	3.09
8	7	0.24	2.29	0.14	2.90
9	8	0.27	2.19	0.17	2.75
10	9	0.30	2.11	0.19	2.62
15	14	0.40	1.87	0.29	2.24
21	20	0.48	1.71	0.37	2.00
25	24	0.52	1.64	0.41	1.90
31	30	0.56	1.57	0.46	1.79
41	40	0.61	1.48	0.52	1.67
61	60	0.67	1.39	0.59	1.53
121	120	0.76	1.27	0.70	1.36

Failure of the warning limit will cause a warning to be printed for every succeeding measurement type, until the MC-Precision Option is successfully passed. Failure of the action limit will cause the system to not allow assays until the MC-Precision Option is successfully passed or a warning limit level is achieved. This test may be avoided by selecting a nonpositive time for the repetition rate.

INTRODUCTION

It might seem desirable to have calibration solutions spanning the measurement range of the instrument (5-500 g/L). However, it is generally impractical to do so. Below about 100 g/L the statistical precision becomes poor enough to require excessively long running times to obtain a meaningful calibration precision (0.1% RSD). Above 400 g/L there can be problems with keeping the plutonium in solution. The user should also note that extensive evaluations exist in the literature; not every facet of the instrument's performance requires frequent repetition.

The physics of the measurement does not require the calibration materials to span the range of the instrument for every calibration attempt. Indeed, a single point does provide a good calibration *if the concentration of the standard is known accurately*. It is recommended that a minimum of two solutions of different concentration be used to calibrate. This can provide a quality check on the accuracy of the concentration claimed for the standards.

The user should be aware of the potential for correlations if a straight-through or background measurement is used for more than one calibration measurement of one or more standards. A better calibration can often be obtained with more measurements and more standards.

DATA ACQUISITION

Make a new background measurement.

Before measuring the standards, make a straight-through measurement. Count for at least 2000 s for each transmission source. We suggest that the user attain measurement uncertainties of approximately 0.1% for each of the normalized net peak areas at 122.1 and 121.1 keV. The fixed times in the parameter file may have to be changed to allow this.

Acquire data from each calibration solution standard. Use the Calibration Option under the long menu. The Calibration Option will request input of the plutonium concentration.

PLOT DATA

Plotting the data can illustrate if there are correlations or trends. The plot should include each result, not average results.

PLOT DATA (cont.)

The autocycle runs under the Calibration option produce an average value for the calibration constant. This result should be independent of sample, concentration, or operator.

Outliers may indicate an incorrect standard value for the claimed concentration, a transcription error, or variability in sample-vial dimensions.

CALIBRATION HISTORY

Date:____

Operator:____

Comment:____

Concentration	±	Number of measurements	Calibration Constant

CALIBRATION HISTORY
(cont.)

Date:______________________________
Operator:____________________________
Comment:____________________________

Concentration	±	Number of measurements	Calibration Constant

CALIBRATION HISTORY
(cont.)

Date:______________________________
Operator:____________________________
Comment:____________________________

Concentration	±	Number of measurements	Calibration Constant

INTRODUCTION

In this appendix, we list additional information about error messages, problems solved during development, and (maybe) other useful hints.

MULTICHANNEL ANALYZER

The MCA can be set with internal jumpers to multiple addresses. This system assumes the factory default. If the computer has problems finding the MCA, the software will offer the choice to switch to the second address. This is not used in the K-edge software.

If the communications between the MCA and computer have a problem, reset both by turning off the power. If the communications problem occurs twice, a hardware failure is indicated

COMPUTER

The computer sometimes locks up; the symptom is that the keyboard will not respond to any command (such as NUM LOCK).

The computer can be sometimes be unlocked bv pushing the CTRL, ALT, and DEL keys simultaneously. If this does not unlock the computer, then push the computer front panel switch to turn the power off. Wait 10 s after turning the power off to allow the disk drive to stop. Then turn the power ON and wait for the operating system to get started.

DIGITAL STABILIZER

If a problem is suspected with the stabilizer, check the switch settings and computer interface cable. Be sure the *manual/remote* switch is set to remote.

The Canberra 8232 stabilizer can lock up. In this condition, it does not adjust the gain and zero. It does not respond to any front panel buttons. Turning its power off and then on will reset it. This can be done by pulling it 5 cm out of the NIM bin and then pushing it back in, without turning the NIM bin off.

If the digital stabilizer does not hold the peaks to the peak channels, the stabilizer may not be working. This is usually indicated when the push button SET and INCR in the front panel do not change the indicator LEDs, this means that the

DIGITAL STABILIZER (cont.)

stabilizer is locked up. To unlock it, remove the unit from the NIM bin momentarily. This should unlock the unit.

The initial adjustment of the system gain and zero to place the gamma-ray peaks into the desired channels is difficult. After the initial adjustment, the system should not require a change unless the detector, ADC, or amplifier is changed. In that case, we suggest that the operator manually set the ^{75}Se source into position using the source control interface chassis. Then turn the stabilizer switch on the front panel to manual mode and turn the zero and gain switches to off. Acquire a spectrum using the Canberra MCA program. Adjust the amplifier gain to fix the 279.528-keV peak in channel 3893. Adjust the ADC zero to fix the 88.036-keV peak in channel 1157. Repeat the gain and zero adjustment until the two peaks are within two channels of the correct channels. Turn the stabilizer switch from manual to remote (this will override the gain and zero switches). Check the first KED measurement to verify that the centroids pass the diagnostic tests. If they do not, repeat this procedure.

GENEVA MECHANISM

The KED program can be used with no communication to the Geneva mechanism interface. Start the program with the additional command, -G, in the subdirectory \tokai.

c:\tokai>**KED -G{return}**

The Geneva mechanism interface can be used in a stand-alone mode. See the Diagnostic Software section in the Troubleshooting appendix for a description of the test program GT.

MEASURED STANDARD DEVIATION EXCEEDS EXPECTED VALUE

This problem can have several causes.

(1) During the initial testing in 1979, the system showed an underlying instability of 0.2%.

(2) If a transmission source is loose in its holder, the excessive standard deviation might be seen in only one of the transmission values.

MEASURED STANDARD DEVIATION EXCEEDS EXPECTED VALUE (cont.)

(3) The uncertainty in the actual standard deviation of n results depends on n. If $n < 25$, perhaps try again with a larger value.

$$\sigma(\sigma) \quad \frac{1}{\mathrm{sqrt}[2(n-1)]}$$

(4) Perhaps the sample is changing. Bubbles or precipitation in the liquid can cause results to vary.

CORRELATED RESULTS

The use of a single straight-through measurement for several sample assays is common practice. Note that this results in correlated values for those results that share the same straight-through measurement. If the uncertainty in the straight-through measurement contributes half of the uncertainty in the assay, a plot of the results shows interesting bias trends. This "problem" seems to be rediscovered by each new user. We recommend the use of very long straight-through measurements.

TEMPERATURE EFFECTS ON DENSITY

The K-edge densitometer does not measure the sample temperature. Therefore a correction for the effects of temperature is not performed. A measurement of a sample with a temperature much greater than room temperature might appear to be biased if the result is applied to tanks at room temperature. If this situation is encountered, the operator must correct for the density variation because of temperature differences.

DIAGNOSTIC SOFTWARE

Some specialized test programs have been built for testing specific features used in the large KED program.

(1) GT is a program to test the parallel interface to the Transmission Source Geneva Mechanism. To use it, first exit the main program KED. Then switch to the subdirectory \okai\test and type gt.

Name-GT gt -- Geneva Mechanism Test Program

Synopsis. gt [-123] [-m] [-a] [-l[*position*]] [-p[*position*]]

Description. *Gt* provides the user with a way to control the Geneva Mechanism. The Computer/Manual toggle on the Geneva Mechanism must be in the Computer position to enable computer control.

A PC may have up to three parallel ports installed. Generally, one of these is connected to a printer. The Geneva Mechanism connects to the PC through one of the available parallel ports (LPT1, LPT2, or LPT3). The user tells *gt* which port to use by selecting one of the port options: -1 for LPT1, -2 for LPT2, or -3 for LPT3. If none of the ports are specified, LPT1 is used by default.

The Geneva Mechanism motor can be controlled directly by the *-m* option. When selected, this option will turn on the motor immediately. The motor will continue running until the user hits any key. The position lights can be activated to track the motor while it is running by using the *-a* option together with the *-m* option.

The Geneva Mechanism position lights may be controlled directly by the *-l* option. An explicit position (1, 3, or 5) may be selected using *position*. If no *position* is specified, position 1 is used by default. When selected, this option will turn on the light immediately. The light will remain on until the user kits any key.

The Geneva Mechanism motor may be sent to a particular position using the *-p* option. An explicit position (1, 3, or 5) may be selected using *position*. If no *position* is specified, position 1 is used by default. When selected, this option moves the motor to the selected position; the position lights track the motor as it moves.

Examples.

gt -?	Displays a usage message.
gt -p3	Using LPT1 Geneva Mechanism moves to position 3 (^{57}Co source).
gt -2 -p3	Using LPT2 Geneva Mechanism moves to position 5 (blank source).
gt -2 -m	Using LPT2 turns on motor (until user hits a key, stopping motor).
gt -2 -m -a	Same as previous example but also turning on position lights as motor moves.
gt -3 -l1	Using LPT3 turn on light for position 1 (^{75}Se source) (until user hits a key turning the light off).

(2) PIO is a program to test the parallel I/O ports. To use it, first exit the main program KED. Then .....

(3) DST is a program to test the digital stabilizer communications. To use it, first exit the main program KED. Then switch to the \tokai\test subdirectory and type dst.

Name-DST

dst — Canberra 8232 Digital Stabilizer Test Program

Synopsis. dst [-p[*port*]] [-b[*baud*]] [-e|o|n] [-g|z] [-k[*peak*]] [-w[*window*]] [-r[*range*]] [-s[*state*]] [-v].

Description. *Dst* provides the user with a way to control the Canberra 8232 Digital Stabilizer. The Remote/Manual toggle on the Digital Stabilizer must be in the Remote position to enable computer control.

The Digital Stabilizer connects to the PC through one of the available serial ports (COM1 or COM2). Please note that this requires a custom cable between the Digital Stabilizer and the PC. The user tells *dst* which port to use by selecting the *-p* option. An explicit port (1 or 2 for COM1 or COM2, respectively) may be selected using port. If no port is specified, COM1 is used by default. The baud rate is selected using the *-b* option. Baud rates of 300, 1200, 2400, and 9600 are supported. If no baud is specified 300 is used by default. The parity is selected using either the *-e*, *-o*, or *-n* options to choose even, odd, or no parity, respectively. If no parity is selected, even is used by default.

Description (cont.)

The user chooses to communicate with either the Gain or Zero controls of the Digital Stabilizer by selecting either the *-g* or *-z* option, respectively. If neither is specified, Gain is used by default.

Dst always gives the current settings of either the selected Gain or Zero. If the user chooses to set one of the settings, *dst* will also read back the revised settings. The peak may be set using the *-k* option. Possible *peak* values are 0 to 19 999. The window may be set using the *-w* option. The range may be set using the *-r* option. Possible *range* values are 0 (for Full), 1 (for Half), 2 (for Quarter), or 3 (for Eighth). The state may be set using the -s option. Possible *state* values are 0 (for Off), 1 (for Hold), or 2 (for On).

Verbose detail of the serial communications between the Digital Stabilizer and the PC may be enabled using the *-v* option. The option is primarily tor debugging purposes.

Examples

dst -?	Displays a usage message.
dst	Using COM1 at 300 baud with even parity, reports current pain settings.
dst -b9600 -o	Using COM1 at 9600 baud with odd parity, reports current gain settings.
dst -p2 -n -z	Using COM2 at 300 baud with no parity, reports current zero settings.
dst -n -z -k1233	Using COM1 at 300 baud with no parity, reports current zero settings, sets the zero peak to 1233, and reports the modified zero settings.

(4) T100S - is a program to .... To use it, first exit the main program KED. Then .....

(5) DB_DUMP is a program to read and print the KED database, KED DB.DAT, which contains the background and straight-through results. To use it, first

Examples (cont.)

exit the main program KED. To send output to the printer use

c:\tokai>**DB_DUMP KED_DB.DAT >PRN**

The KED program can be started with some features disabled. If you do not want to use the interface to the Geneva mechanism, add the option -G to the command line that starts the program.

c:\tokai>**KED -G**

To override the diagnostic tests, which block certain actions after a test failure, add the option -O to the command line that starts the program:

c:\tokai>**K') -O**

ERROR MESSAGES

We have attempted to make the error messages complete and self-explanatory. Please contact the safeguards assay group at Los Alamos if you need help: Jim Sprinkle (505)-667-4181 or Walt Hansen (505) 667-8818.

Two levels of error/warning messages are used in the KED program. Blue messages are not as serious as red messages. Some blue messages inform the user that the program is busy, while some appear as warnings. A warning limit is chosen such that occasional false alarms occur. A false alarm rate of 2-5% is considered acceptable. Red messages indicate a more serious problem. Red messages usually require the user to perform a repair or adjustment. The limits for red messages are chosen so that false alarm rates are less than 0.5%.

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Title: WIDER AVAILABILITY OF PARMILA AND RECENT IMPROVEMENTS TO PARMILA

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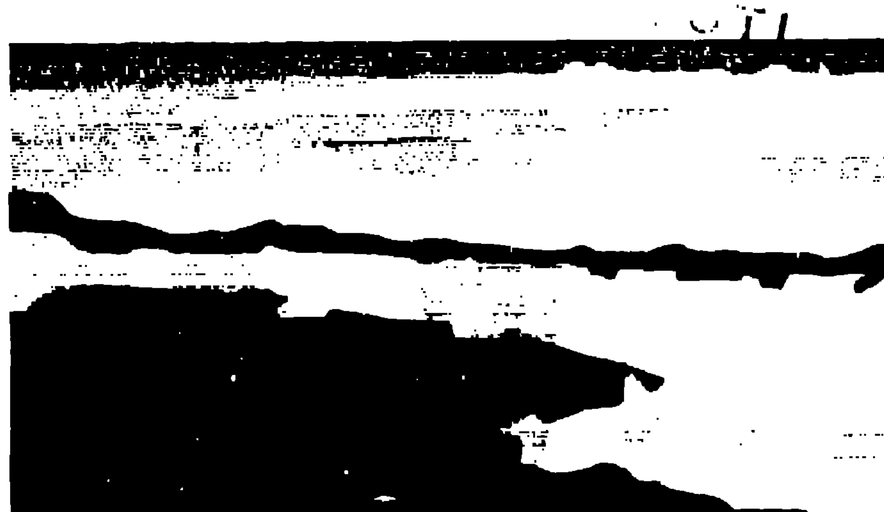

MASTER

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WIDER AVAILABILITY OF PARMILA AND RECENT IMPROVEMENTS TO PARMILA [a]

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ABSTRACT

PARMILA (Phase And Radial Motion in Ion Linear Accelerators) is a drift-tube linac (DTL) ion-beam dynamics code. Over its long life, many versions have developed. The Los Alamos Accelerator Code Group distributes a version, for which a manual[1] is available. Unless otherwise specified, all mentions of PARMILA in this document refer to that LAACG-distributed version. Until recently, this documented and distributed version functioned only under CTSS. Users who wished to run on a different operating system needed to convert the code themselves. PARMILA now operates under UNICOS, a much more widely available CRAY operating system, and under VAX/VMS. This paper describes some new features of the code, and gives directions for obtaining the manual and the UNICOS and VMS versions of the code.

INTRODUCTION

Reference 1, the PARMILA manual, describes the major features of PARMILA as it is distributed by the LAACG. Unless otherwise specified, all mentions of PARMILA in this document refer to the LAACG distributed version. This paper emphasizes features that have been added since the first version of that report was published in 1990, and those that are not well documented. The 1992 revision to the manual was minor. The new features include the ability to scale data from SUPERFISH, availability of a second linac generation subroutine, two new output files giving emittances and power requirements, and the ability to handle comments in the input file.

We also describe a post processor for PARMILA, named NBFAM6.

[a]Work supported by U S Department of Energy, Office of Energy Research: Office of High Energy and Nuclear Physics, Office of Basic Energy Sciences, Office of Fusion Energy, Office of Superconducting Super Collider, and Scientific Computing Staff

SCALED SFDATA INFORMATION

A table of information generated by running the cavity code SUPERFISH[2,3] provides the basis for generating a linac. PARMILA now has the ability to scale information in an SFDATA table based on SUPERFISH analysis of cells having one resonate frequency to a different design frequency[4]. In order to utilize this feature, the user must specify the reference frequency for which the SUPERFISH runs were done, FREQREF. The fifth data element after the LINAC label is set equal to the value of FREQREF, in megahertz. Then PARMILA multiplies each shunt impedance, Z, in the SFDATA table by the square root of the ratio of the design frequency to the reference frequency. (The design frequency is the third data element following the LINAC label, as described in the manual.) If no value for FREQREF is given, PARMILA assumes it to be equal to the design frequency. This scaling is done in the main program, and is independent of the linac generation routine selected for use (see next section).

CHOICE OF ROUTINE TO GENERATE LINAC

PARMILA now contains two routines that the user can select to generate the linac. The two routines have somewhat different capabilities, and even for the same input data, they generate slightly different linacs. The new routine, which is named GENLAT1 in PARMILA, is similar to the linac-generating routine used in the AT-1 PC version of PARMILA. It is the routine that is called by default when all the cells for which SFDATA information is provided are symmetric.

The old routine, GENLIN2, can deal with asymmetric cells, and is called automatically if any asymmetric cells are represented in the SFDATA input. If the SFDATA is for a symmetric cell, entry number 8 equals zero ,and entries 9 and 10 are ignored but must be present for spacing. For an asymmetric cell, entry number 8 is nonzero, and it, along with entries 9 and 10, gives the characteristics of the second half of the cell. See reference 1 for details. GENLIN2 also generates a file of power requirements, described below.

In order to use GENLIN2 when all cells are actually symmetric, an artificial value for SFDATA entry 8 is used. Set entry number 8 in the SFDATA information for at least one cell equal to 9000.0. PARMILA will reset it to zero but will set a flag to cause GENLIN2 to be called.

The new routine, GENLAT1, allows an automatic ramp of phase, either with or without ramping E0. To ramp phase only, set vv(30) [b] following a TANK label to 1, and vv(5) following the TANK label to less than 0 1e10. To ramp both phase and E0, set vv(5) equal to 1.0e10 and VV(30) to 1. For ramp of E0 only, see the manual. (The E0 only ramp capabilities are similar in GENLAT1 and GENLIN2.) A 10 cm delay in the phase ramp is programmed into GENLAT1. It can be changed by changing the numeric value in one "if" statement that checks

[b] vv(n) is the nth data element following its associated label

"(gnlen .le. 10.00)" and recompiling. Similarly, the phase limit can be changed by changing the value assigned to SPMINV in the routine and recompiling. This assignment occurs immediately after the comment "generate linac".

NEW OUTPUT FILES

Two additional output files not documented in the manual are now available. The file EMITT contains 100%, 90%, and rms emittances, as well as α and β in the x-xprime, y-yprime and phase-energy phase space planes at each cell, and the number of particles that have not been lost to that point. The file is written by subroutine EMIT.

POWFILE contains the power requirement in megawatts for each cell and the cumulative power requirement to that cell in the tank. It is written by subroutine GENLIN2.

COMMENTS

Data on a line that starts with a COMMENT label will now be ignored. This permits comments to be included in input files.

POST-PROCESSOR

A post processor named NBEAM6 has been locally available for use with the version of PARMILA but has not been documented. It is now also available for use with UNICOS It provides graphical and tabular descriptions of a beam from PARMILA, taking the beam particle coordinates from a file named by the user. Histogram plots of the beam particle distributions in x, xprime, y, yprime, phase, and energy are available, either with or without Gaussian curves fitted to the distributions. Figure 1 shows an example histogram plot with fitted Gaussian.

Scatter plots in each of the phase space planes are available. An example is given in figure 2. Tabular descriptions of either a set of nine percentages of the beam (a "full range analysis") or of a single percentage of the beam specified by the user are presented in the output file named FORT.4. The values of the step, mean, standard deviation, and third moment associated with the fitted Gaussian curves are given in a file named OUTPUT. The program makes use of the proprietary graphics software, DISSPLA

Use of the program is interactive, and the user is prompted for input. An example interactive session follows.

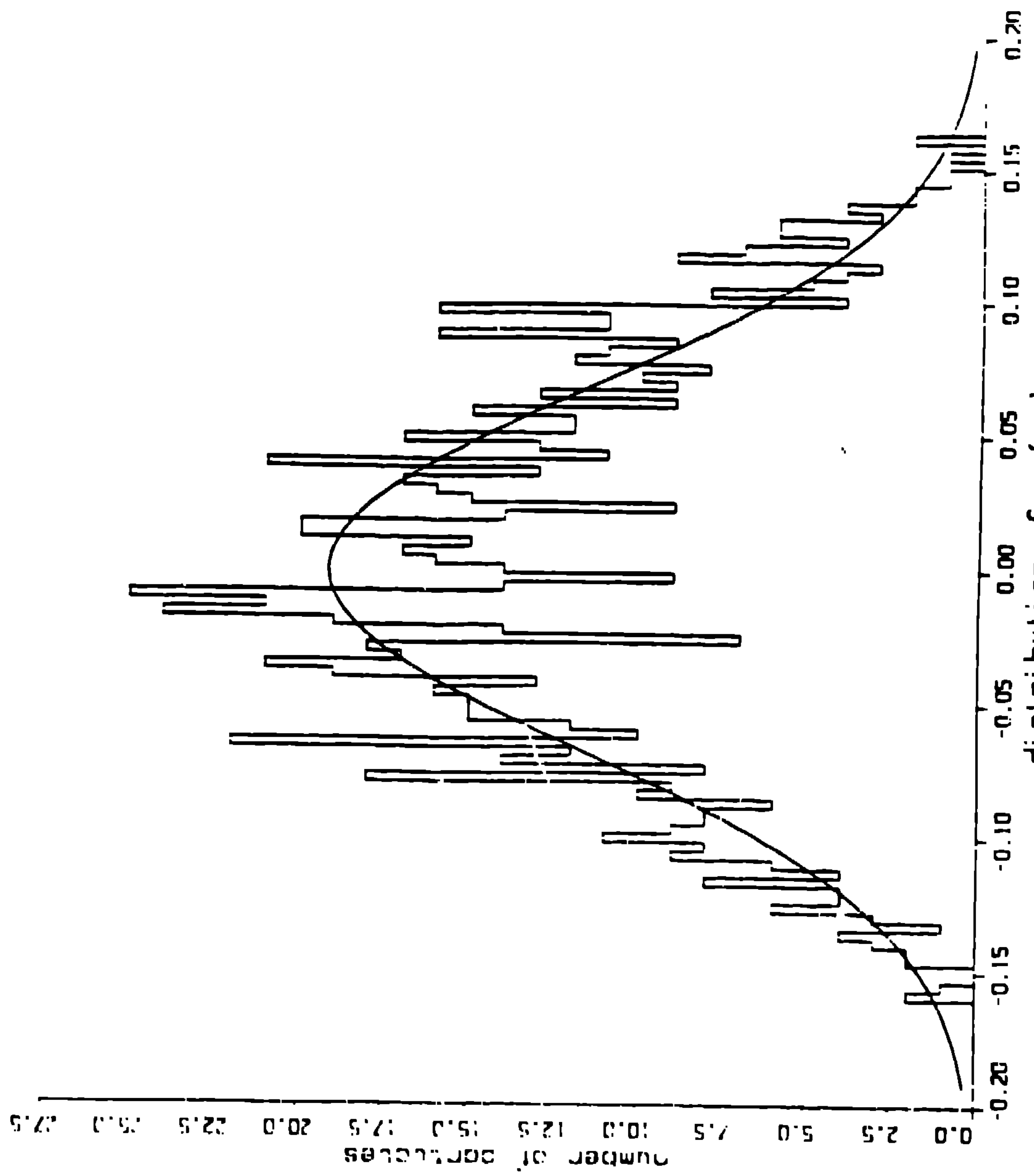

Fig. 1. Histogram plot of particle distribution in y, with fitted Gaussian.

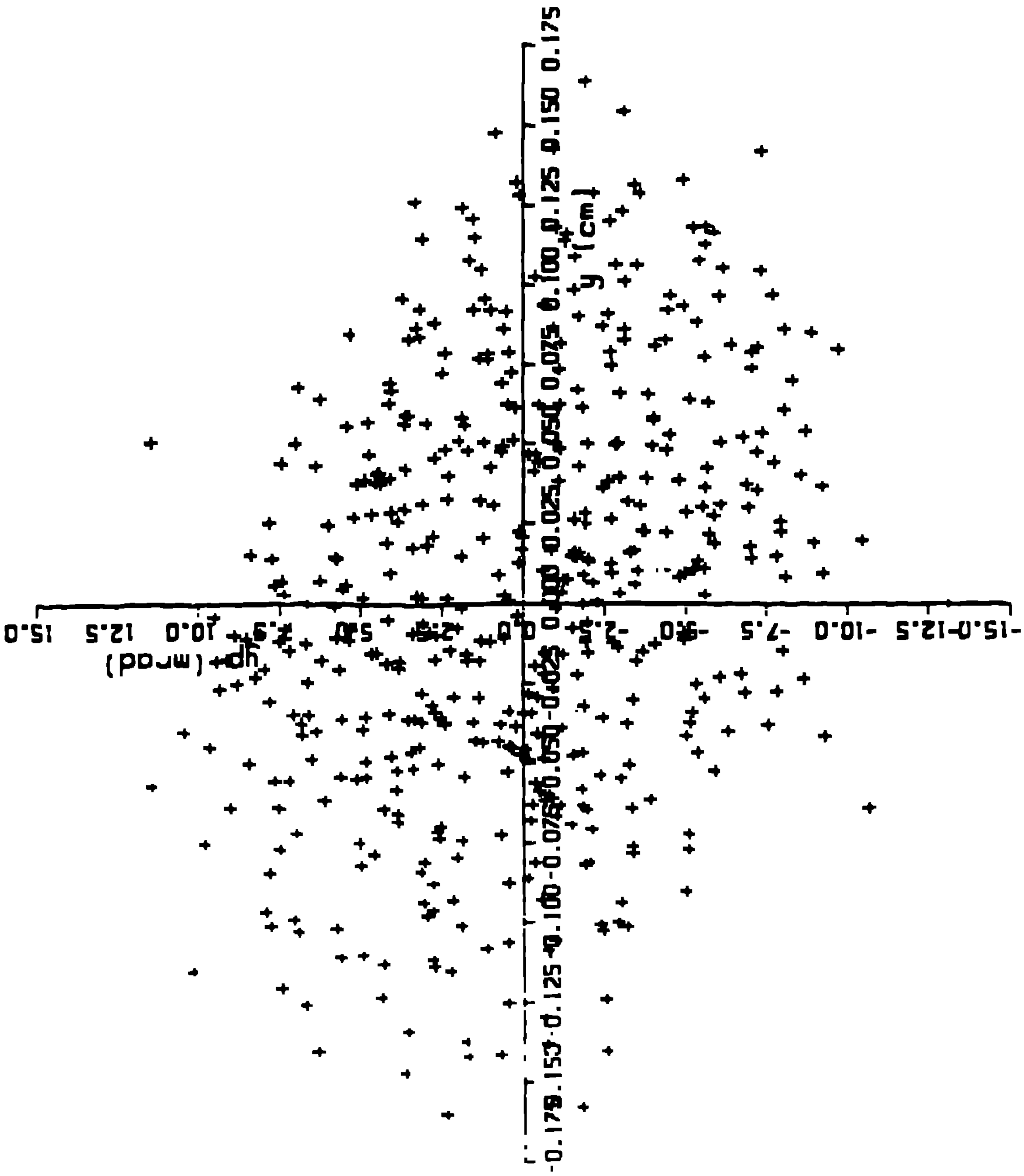

Fig. 2. Phase space distribution in y vs. y prime.

```
 give coordinate input file name.
tape25
 what is dimension of cord on input file?
6
 give first four letters of type of particle.
try <prot>,<deut>,or <hmin> or <stop> to exit code.
hmin
want to use synch energy-synch phase <y> <cr>?
if <cr>, will use wbar-pbar calculated in this code.
y

 read from tape5     synch energy       5.0504 mev
                     synch phase       -0.6981 radians

do you want a full range analysis? <y> or <cr>
y

parmila short input file

 do you want plot output ? <y> or <cr>
y

do you want histograms plotted? <y> or <cr>
y
 do you want plots of fitted gaussian distribution? <y> or <cr>
y
to change distribution limits enter any or all xl,xpl,yl,ypl,phimin,phimax,
wlow,whigh,npar. namelist format. namelist name=limits
 $limits$
 do you want sample emittance plots? <y> or <cr>)
y
to change plot limits enter any or all xmx,xpmx,ymx,ypmx,wmx,pmx
use namelist format. namelist name is maxs
 $maxs$
 plot    done.  pages =    11.  words =     10517
 graphics cl = u
 END OF DISSPLA 11.0 9003, DRIVERS 9003 -- 20519 VECTORS IN 10
 PLOTS.
 RUN ON 1/12/93 USING SERIAL NUMBER 2545 AT LOS ALAMOS NATIONAL
 LABORATORY
 PROPRIETARY SOFTWARE PRODUCT OF COMPUTER ASSOCIATES, INC.
 9763 VIRTUAL STORAGE REFERENCES; 7 READS; 0 WRITES.
```

CONCLUSIONS

The manual, the UNICOS version of PARMILA, or the VAX/VMS version can be obtained by sending a request to The Los Alamos Accelerator Code Group by one of the means given below.

Mail request to:

Los Alamos Accelerator Code Group (LAACG)
Mail Stop H825
Los Alamos National Laboratory
Los Alamos, New Mexico 87545
USA

Phone:

(505) 667-9131

E-Mail:

laacg@lanl.gov

Please include the following information with your request: code and/or documentation requested, your name, organization, address, phone number, fax number, and E-mail address, and the computer and operating system on which you intend to use the program.

The LAACG is restricted in its dealings with persons from countries on the U.S. Department of Energy's sensitive countries list. The code group can send such persons documentation, but they must request software from the Energy Science and Technology Software Center (ESTSC). For those who must request software from the ESTSC, the center can be reached as follows:

Phone: (615) 576-2606
Fax: (615) 576-2865
Mail: Energy Science and Technology Software Center
P.O. Box 1020
Oak Ridge, TN 37831
USA

The Los Alamos Accelerator Code Group is able to send the manual to requestors in sensitive countries.

References

[1] G. Boicourt and J. Merson, "PARMILA Users and Reference Manual," Los Alamos National Laboratory report LA-UR-90-127 (January 10, 1990, revised September 25, 1992)

[2] M.T. Menzel and H.K. Stokes, "User's Guide for the POISSON/SUPERFISH Group of Codes," Los Alamos National Laboratory report LA-UR-87-115 (January 1987)

[3] Los Alamos Accelerator Code Group,"POISSON/SUPERFISH Reference Manual," Los Alamos National Laboratory report LA-UR-87-126 (January 1987)

[4] Thomas P. Wangler, private communication, October 1991

[5] George H. Neuschaefer, private communication, December 21, 1992