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LEAST-SQUARES RESOLUTION OF GAMMA-RAY SPECTRA IN ENVIRONMENTAL SAMPLES

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LEAST-SQUARES RESOLUTION OF GAMMA-RAY SPECTRA IN ENVIRONMENTAL MONITORING

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ABSTRACT

The use of ALPHA-M, a least-squares computer program for analyzing NaI(Tℓ) gamma spectra of environmental samples, is evaluated. Included is a comprehensive set of program instructions, listings, and flowcharts. Two other programs, GEN4 and SIMSPEC, are also described. GEN4 is used to create standard libraries for ALPHA-M, and SIMSPEC is used to simulate spectra for ALPHA-M analysis. Tests to evaluate the standard libraries selected for use in analyzing environmental samples are provided. An evaluation of the results of sample analyses is discussed.

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SECTION 1

INTRODUCTION

The emphasis on monitoring the environment for radiological impact is growing with the increased use of nuclear power. Increased nuclear power production requires greater production from all aspects of the uranium cycle, from mining and milling to spent fuel reprocessing. One of the most economical and wide-ranging analytical tools for environmental monitoring is gamma spectroscopy. However, accurate quantitative information from gamma-ray analysis is difficult to obtain, and data reduction requires a sophisticated approach to produce reliable results.

The basic purpose of this report is to evaluate a standard least-squares computer program for analyzing gamma-ray spectral data obtained with NaI($T\ell$) scintillation detectors. A modified version of ALPHA-M (developed by E. Schonfeld) has been prepared and tested to determine its capabilities and limitations for environmental monitoring. This program is presented in Appendix A.

Certain procedures for evaluating the performance of ALPHA-M in an individual laboratory program, detailed in this report, should be completed before adopting ALPHA-M for routine analytical work.

Since the audience for a report of this nature is generally quite broad, it is difficult to select the subjects that should be covered. The material has been written for a person with at least a B.S. degree in the physical sciences and a limited amount of experience in the fields of radiochemistry and gamma spectroscopy. In an attempt to discuss the full range of the radioanalytical problem, a section (Section 4) on gamma spectroscopy has been included. Section 4 is also an introduction for new personnel to the problems of gamma spectroscopy and quantitative radionuclide analysis. The experienced spectroscopist may wish to skip Section 4 and turn directly to Section 5, which contains instructions for using ALPHA-M. Section 6 describes methods for evaluating the library standards, background fluctuations, and program processing options. The program ALPHA-M, its flowcharts, and other related material are contained in Appendix A.

SECTION 2

CONCLUSIONS

The least-squares analysis program ALPHA-M can be used successfully to quantify NaI(Tℓ) spectra of environmental samples. Many gamma-emitting radionuclides can be quantified at activity levels of about 10 pico-Curies per liter (pCi/ℓ) or less, depending on counting time, at a confidence level of 95 percent. The least-squares analysis method is an effective environmental monitoring tool, and program operation is relatively inexpensive in terms of counting instruments and actual analyst time.

SECTION 3

RECOMMENDATIONS

Quantitative analysis of complex gamma-ray spectra taken with NaI(Tℓ) detectors should be performed with a weighted least-squares fitting program such as ALPHA-M. The user of such a program should study carefully the theoretical model (including weighting scheme, standards compatibility, and background interferences) before he uses the program for routine analyses. The user should also provide for continuous performance testing and evaluation during routine use of the program to help prevent the production of erroneous data.

Although ALPHA-M is now a valuable tool in environmental monitoring, areas for further development could be investigated: (1) possible modifications to improve the gain and threshold shift procedure for environmental samples, where counting statistics are often poor; (2) possible modifications in the rejection procedure to compensate better for imprecise determinations of low activity levels of radionuclides so that possibly valid data is not discarded; (3) development of techniques to better handle highly correlated spectra of certain radionuclides (see Section 6.3); and (4) development of better criteria than the residuals and chi-square tests to indicate the validity of the program results.

SECTION 4

GAMMA SPECTROSCOPY

4.1 GENERAL

Gamma rays are a type of electromagnetic radiation characterized by zero rest mass and no electrical charge. They differ from visible light only in having much shorter wavelengths (i.e., much higher energy). Gamma rays arise from transitions of nucleons between nuclear energy levels, just as optical spectra arise from transitions of electrons between electronic energy levels.[1,2] Although energy adjustments in the atomic nucleus that lead to gamma-ray emissions usually occur after the emission of alpha or beta particles, there are some cases in which gamma-ray emission occurs without an accompanying alpha or beta emission. For example, ^{54}Mn and ^{85}Sr emit only gamma rays.

A single radionuclide may emit one or more gamma rays, depending on the variableness of prior alpha or beta emission energies. Although the energy of these gamma rays is characteristic of a particular radionuclide, a particular radionuclide is not necessarily the only source of a specific gamma-ray spectral line. For example, ^{226}Ra emits a gamma ray with an energy of 186,000 electron volts (186 keV), but ^{235}U and several other radionuclides also exhibit a 186-keV emission. Thus, one difficulty of gamma spectroscopy is the assignment of gamma-ray lines to particular radionuclides.

4.2 INTERACTIONS OF GAMMA RAYS WITH MATTER

The practical energy range for gamma spectroscopy is from a few thousand to a few million electron volts. Within this energy range, there are basically three processes by which gamma rays may interact with matter: the photoelectric effect, the Compton effect, and pair production.[1-4] The relative importance of these three modes of interaction to the absorption process is a function of the atomic number of the absorber and the energy of the incident gamma ray. This relationship is shown graphically in figure 1.

The photoelectric effect occurs when a gamma ray transfers all its energy to a bound orbital electron. The electron uses a portion of this energy to overcome its binding energy and assumes the remainder as kinetic energy. This process cannot occur with a free (unbound) electron because a third body, the nucleus, is required to conserve momentum.

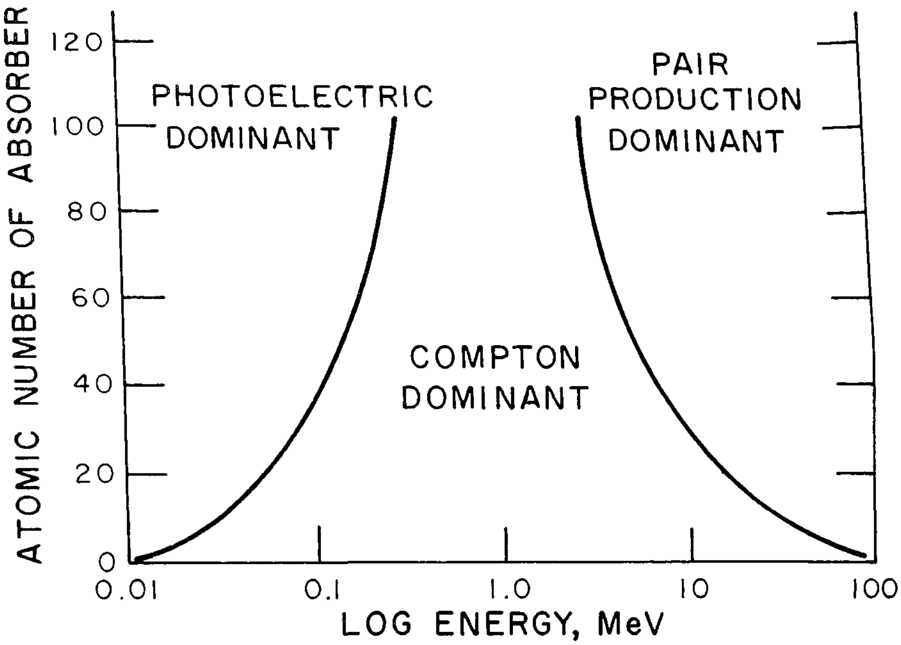

Figure 1. Interaction processes.

Therefore, a more tightly bound electron has a higher probability of undergoing the photoelectric process. When the incident photon energy significantly exceeds the K- or L-shell binding energies, the probability of photoelectric interaction in the outer shells is negligible. The removal of an electron from a low-lying orbit leads to higher-energy electrons dropping down to fill the vacancy. These excited atoms lose energy by emitting characteristic X-rays when the electrons drop down to fill lower-lying orbits.[2]

For gamma photons having energies much greater than the electron-binding energies, the photoelectric process is not favored. Rather, the photons are scattered when they interact with the electrons as if the electrons were free and at rest. This process is called the Compton effect, or Compton scattering, and is the dominant mode of interaction at energies of about 1 MeV. In the scattering process, the gamma photon transfers a portion of its energy to an electron as the photon is deflected from its original path.[2,4]

If the path of a single gamma photon in a scintillation detector were observed, the photon might be seen to have several Compton interactions followed by either a photoelectric interaction or escape of the scattered photon from the crystal. Since Compton scattering generally involves the outer electrons of an absorber atom, a significant number of X rays are not produced except in absorber elements of low atomic number.[1]

For energies above 1.02 MeV, pair production, the third mode of interaction of gamma rays with matter, becomes increasingly more important. In pair production, a gamma photon passing through the field of a nucleus disappears with the creation of an electron-positron pair. The kinetic energy of this pair is equal to the difference between the incident photon energy and the rest mass energy (1.02 MeV) of the two particles. The emitted particles rapidly dissipate their kinetic energy by ionization or radiative processes. When the kinetic energy has been dissipated, the positron that has an available electron is annihilated, producing two annihilation photons, each having 0.51 MeV energy. These photons, which are emitted at 180 degrees with respect to each other, can also undergo Compton scattering and photoelectric interaction to produce a complex spectrum.[2]

The entire process of gamma-ray absorption can be described as an exponential attenuation of the incident beam. That is, the number of photons remaining in the beam decreases exponentially with the distance of penetration into the absorber. This can be written

$$I = I_0 e^{-\mu x}, \qquad (1)$$

where I_0 = incident beam intensity,
I = beam intensity at distance x,
μ = linear absorption coefficient of the absorber,
x = distance penetrated.

The linear absorption coefficient, μ, sums all the coefficients for the photoelectric, Compton, and pair-production processes.[4] Equation (1) assumes the idealities of a point source and a "thin" absorber. Since, in reality (i.e., in environmental samples), such ideality does not occur, a proportionality constant must be determined to relate the ideal case to the observed data. This is done by preparing a known source in the exact geometry to be used for sample analysis.

4.3 CHARACTERISTICS OF GAMMA-RAY SPECTRA

Gamma-ray spectra, obtained with a multichannel analyzer and an NaI scintillation detector, have several possible characteristic features: (1) photopeaks, (2) Compton area, (3) escape peaks, (4) annihilation peak, (5) sum peaks, and (6) nongamma components (such as bremsstrahlung). All six features can lead to a complicated spectrum for even a single radionuclide having multiple emissions; thus, spectra of radionuclide mixtures can become very complex. An experimental NaI(Tℓ) spectrum is shown in figure 2.

The photopeak, which results from the total absorption of the energy of the gamma photon in the scintillation detector, is the most important feature of the spectrum because its amplitude and intensity are direct measures of the energy and intensity of the incident monoenergetic gamma ray beam. The width of the photopeak reflects the energy resolution of the spectrometer system, and the fraction of total counts appearing in the photopeak is a function of the detector volume. This fraction of total-absorption events is much larger than predicted by theory for photoelectric interaction because of the high probability of all photon interaction processes, such as the photoelectric effect and Compton scattering, occurring during the collection time of the scintillation detector, producing only one detector pulse. Therefore, the single detector pulse reflects the sum of all the successive Compton events and the final photoelectric process.[5,6]

The Compton area of the spectrum stretches from essentially zero energy to a maximum energy value indicated as the Compton edge in figure 2. This area, known as the Compton Continuum, arises from scattered gamma photons escaping the detector before undergoing complete energy transfer to the crystal.[4,5] Because the possible number of different Compton interactions is quite large, a broad energy spectrum results. The Compton portion of the spectrum varies with the energy of the incident photon. However, the Compton Continuum has a definite upper limit known as the Compton edge. This limiting energy value occurs when the incident photon is scattered through an angle of 180 degrees, thereby imparting the maximum kinetic energy to the ejected electron.[4] The value for the Compton edge increases and the Compton Continuum broadens as the incident photon energy increases.

Another characteristic of the Compton area is the back-scatter peak. This peak results from the 180-degree Compton backscattering of gamma rays by the surrounding materials such as the detector shield. The shape and magnitude of this peak are functions of the geometry of the counting system. The intensity of this peak varies inversely with the size of the shield and the atomic number of the shield material. In other words, a large shield will show a substantial reduction in the amount of backscattering because more of the interactions of the gamma ray with the shield will proceed photoelectrically (figure 1). This reduction is achieved because most of the gamma photon energy is dissipated before striking the shield, therefore increasing the probability of the photoelectric effect being dominant.

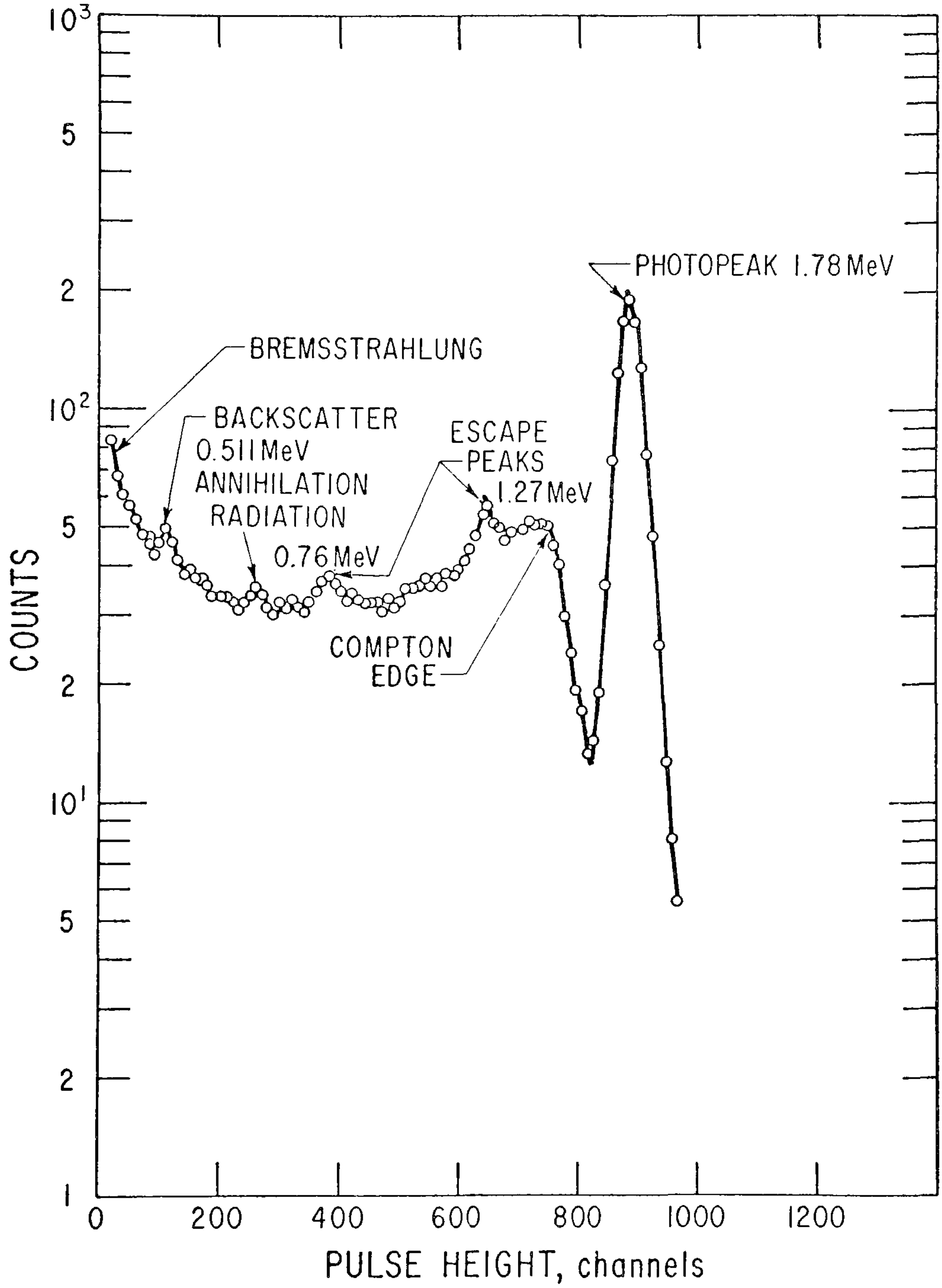

Figure 2. Representative gamma-ray spectrum.

Another feature of the gamma-ray spectrum is the appearance of escape peaks, which are caused by the repeated escape of a discrete amount of energy from the detector. Therefore, an escape peak occurs at a discrete value(s) of energy below the energy of the photopeak (figure 2). The most common escape peak arises from pair production and its associated annihilation radiation. If a positron-electron annihilation occurs near the detector surface but inside the detector, there is a reasonable probability that one of the two annihilation photons, or possibly both, may escape the crystal.[2,4,5] When one annihilation photon does escape repeatedly, a second peak will appear in the spectrum at an energy 0.51 MeV less than that of the photopeak. If both annihilation photons escape the detector, another escape peak will occur at an energy 1.02 MeV less than that of the photopeak. Other escape peaks can arise from the photoelectric interactions of gamma rays with the iodine atoms of the NaI(Tℓ) detector.

If positron-electron annihilation occurs outside the detector, an annihilation photon of 0.51 MeV can penetrate the detector. This behavior can add a small peak, the annihilation peak, in the gamma-ray spectrum at 0.51 MeV.

There is also a possibility that more than one gamma photon may enter the detector simultaneously. If this occurs within the collection time of the detector, the combined light emission will be seen by the photomultiplier tube as a single light pulse. Repeated occurrence of this type of event will lead to a sum peak (figure 3) at higher energy than that of either individual gamma photon.

The common sources of sum peaks are the summing of (1) two gamma photons emitted in cascade from one radionuclide, (2) different gamma photons from a composite sample, and (3) two 0.51-MeV annihilation photons giving rise to a peak at 1.02 MeV. The probability of the appearance of sum peaks is higher when sample activity is higher and a large volume detector is used.[2]

Two other nongamma components that frequently appear in gamma spectra are bremsstrahlung radiation and X rays. Bremsstrahlung radiation is emitted when an electron passes away from the strong, attractive electric field of the nucleus. This phenomenon occurs when high-energy beta particles are emitted from the sample or when pair production has a high probability for a particular gamma ray since the electron produced in pair production decelerates while moving away from the nucleus. X-ray contributions to the gamma spectrum are produced principally by the photoelectric interaction process.[4]

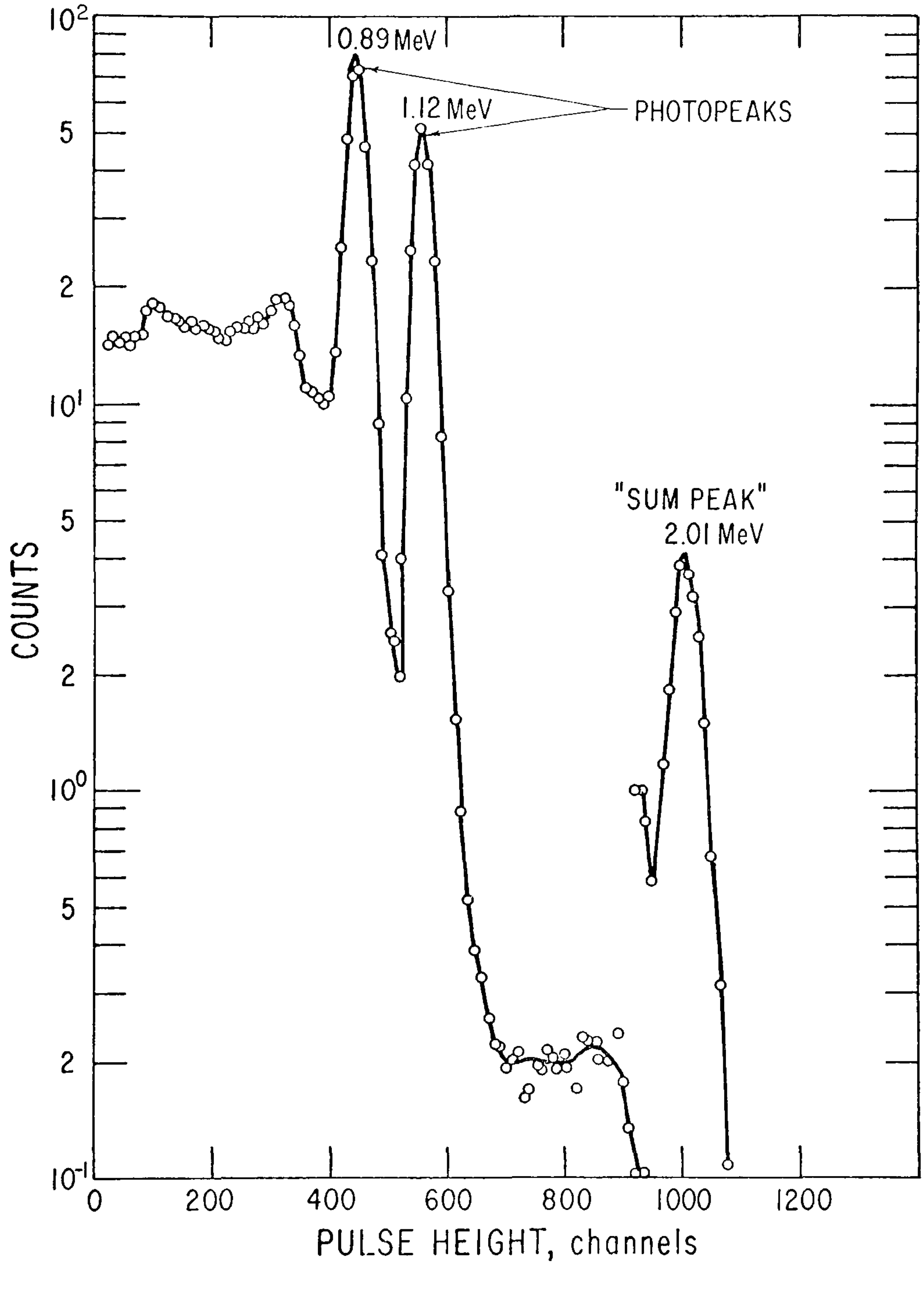

Figure 3. Gamma-ray spectrum with sum peak.

In summary, the peaks often seen in a gamma spectrum result from basic interaction processes. Complications occur when Compton-scattered or annihilation photons escape from the crystal or when other photons are scattered into the crystal from the shielding. This pattern of peaks can become quite complicated when mixtures of radionuclides, such as those contained in environmental samples or reactor effluents, are examined. These spectra can be further influenced by the source-detector geometry, the count rate input to the spectrometer, the size and shape of the detector, and the experimental conditions at the time of analysis.

4.4 THE EXPERIMENTAL PROBLEM--INSTRUMENTAL

A basic system for collecting gamma spectroscopy data consists of a NaI(Tℓ) detector connected to a pulse-height analyzer. The quality of the data depends primarily on the components of the spectrometer. For precise analytical work, standard measurement conditions must be maintained, especially if computer analysis is planned.

An examination of the experimental problems of gamma spectroscopy must begin with the detector. For a reasonable compromise of efficiency and resolution, most environmental work is done with either a 3- by 3-in. or a 4- by 4-in. right-cylinder-shaped NaI(Tℓ) crystal. The crystal is hermetically sealed in an aluminum casing with an optical joint connecting the crystal to a photomultiplier tube.[7,8] Caution must be exercised when using NaI(Tℓ) crystals to prevent thermal or mechanical shock that could fracture the crystal. Such damage could dramatically change the light transmission properties of the crystal. The detector and photomultiplier tube are usually purchased as a system, and both elements contribute to the spectrometer resolution. Resolution is usually defined as the relative width of the photopeak generated by a monoenergetic source of gamma rays (e.g., ^{137}Cs source). Percentage resolution[8] can be calculated by

$$W_{\frac{1}{2}} = \frac{\Delta h_{\frac{1}{2}}}{h_{max}} \times 100\% \quad , \qquad (2)$$

where $W_{\frac{1}{2}}$ = the full peak width at half maximum peak height, % (this resolution is valid only at the energy calculated),

$\Delta h_{\frac{1}{2}}$ = width of photopeak at half maximum peak height, units of energy,

h_{max} = energy value of photopeak.

Some parameters influencing resolution are light production in the scintillator, light collection by the phototube, photocathode electron production, and phototube electron multiplication. Experimental parameters such as temperature, source-detector geometry, and count rate can also vary the detector resolution.

The phototube gain shifts with variations in operating voltage or source count rate. Changes in gain resulting from operating voltage variations can be minimized by using well-regulated power supplies. The magnitude of gain shift with count rate is proportional to the phototube current; usually, an increase in the count rate causes an increase in phototube gain. In environmental work, gain shift with count rate is rarely a problem and would possibly occur only during the counting of high-activity standards.

To minimize problems with voltage-related gain shift, a check source such as ^{137}Cs can be used to readjust the gain between analyses. This calibration can reduce gain variations to less than 0.5 percent, if other factors such as temperature are held constant. The gain shift problem can also be minimized if a source such as ^{241}Am is introduced into the scintillation crystal. Appropriate circuitry can then be installed to automatically adjust the phototube bias to keep the ^{241}Am line at a fixed position in the spectrum.

Once a proper pulse is generated by the detector system, the pulse must be amplified for use in the pulse-height analyzer. The linearity and stability of the amplification system must remain constant with changing experimental conditions (e.g., temperature fluctuations and variations in counting rate, gain, etc.).

One important amplifier problem is zero or threshold shift with count rate. Threshold shift with count rate is caused by pulse pileup; that is, the count rate is so high that circuit capacitance does not have time to discharge completely. Succeeding pulses to the pulse-height analyzer then appear larger than their actual size. This problem can be eliminated by using the "double-differentiating" type of amplifier.[7]

The pulse-height analyzer can be performance-rated on the basis of variables such as its integral and differential linearity, both of which are basically functions of the analog-to-digital converter (ADC).

The integral linearity is the relationship of the input pulse amplitude to the channel position in which the pulse is stored. For example, if the analyzer is calibrated for 5 keV per channel, a 100-keV pulse should appear in channel

20. In general, this relationship will not be linear; that is, there usually will be deviations at very low and very high energies. The integral linearity curve must be adjusted each day by using a multiline calibration source to align the system.[7]

The differential linearity describes the uniformity of channel width over the entire analyzer memory. With newer analyzers, this uniformity is usually better than can be easily measured in the laboratory, but the analyzer performance should be periodically checked to ensure that constant channel width is maintained. This is usually done with a sliding scale pulser.

In summary, a large number of variables influence the quality of data obtained from a gamma spectrometry system. Because these variables have complex interrelationships that are impossible to compute, a set of standard experimental conditions must be defined and rigidly controlled to produce data that can be quantitatively analyzed with accuracy and precision.

4.5 THE EXPERIMENTAL PROBLEM--EXTRANEOUS COUNTS

The most difficult problem in the radioanalytical laboratory is extraneous counts, that is, the problem of isolating the radiation emitted by a specific radionuclide in the sample from that of all other sources. These extraneous counts can originate from two different sources--background radiation or interference from other radionuclides within the sample.[10]

Background radiation usually is determined by measuring a simulated sample or source that is identical to an actual sample except for the relative absence of radioactivity. This technique can simulate counts arising from naturally occurring radioactivity (e.g., ^{40}K and decay products of the ^{238}U and ^{232}Th series), radioactivity in the detectors, cosmic rays, electronic noise, etc. However, this technique assumes that background activity is stable (constant over a period of time) and that the only fluctuations that occur are due to the statistics involved in the radioactive decay process. Actually, background activity often has more variability than predicted by counting statistics.

To reduce background contributions, shielding is necessary. Thick, graded shields of selected lead or steel will measurably reduce background arising from environmental radioactivity. Further reduction in background can be achieved by anticoincidence counting.

Background contributions from environmental sources are exemplified by radon daughters--decay products of the ^{238}U series such as ^{214}Bi and ^{214}Pb. Radon is always present in the laboratory; it can be found in concrete block walls, compressed air, water, and the samples. Therefore, laboratory procedures can only attempt to minimize the effect of radon. Several measures can help reduce background contributions resulting from radon: (1) Air can be exchanged rapidly in the laboratory (five to ten times per hour), (2) water can be boiled or aerated, and (3) compressed air can be supplied from cylinders that are filled more than 30 days before use in the laboratory.

Interference can be caused by other radioisotopes in the sample that are either present originally or that are introduced during sample processing. Errors encountered from contamination during sample processing may be reduced by carrying a "blank sample," a sample having no known activity, through the total analysis scheme. However, in a situation in which more than one radionuclide in the sample is of interest, the multiple components may interfere with each other or may have decay products that interfere and cannot be eliminated. How the ALPHA-M technique handles this problem is discussed in Section 6.3. If the interferents are different elements, chemical separation is possible; if they are the same element, the interferents may be distinguishable by a physical technique, such as a half-life determination.

Overall, extraneous counts generated by interfering radio-activity limit the accuracy attainable in any analysis. Corrections depend on the degree of separation possible and the reproducibility of the separation. Nevertheless, the statistical fluctuations from the interferent will cause errors in the final result just as background variations do.

4.6 QUANTITATIVE ANALYSIS OF GAMMA SPECTRA

To obtain quantitative information from gamma-ray spectral data, the spectral analysis method must attempt to account for several types of problems:[4]

1. Compton interference of higher-energy gamma rays with the photopeaks of lower-energy photons.

2. A multiplicity of photopeaks from different radio-nuclides present in the sample. These photopeaks may overlap one another.

3. Interference from secondary peaks such as escape, annihilation, and sum peaks.

4. Wide variations in the relative activities of the nuclides present.

5. Variations in the detection efficiency for different energy photons.

6. Estimation of errors.

Many techniques for resolving gamma-ray spectra are available, but none can completely meet all these criteria.

One simple approach to quantifying spectral information is the use of a graphical technique, in which a graph of the spectrum is searched for an identifiable, unobstructed photopeak of good intensity. Once found, the same number of channels on either side of the peak are totaled. The baseline is subtracted by extrapolating the baseline from one side of the peak to the other. This method results in an accuracy of only 10 to 30 percent and is limited to levels above 20 to 50 pCi/ℓ. The method cannot readily handle complex spectra or account for small peaks that are hidden by the Compton Continuum of higher-energy radionuclides. Such limitations make the graphical technique almost useless in environmental work.[4]

A second method that is used commonly is spectrum stripping. The basic assumption in spectrum stripping is that a composite spectrum will be the channel-by-channel summation of the spectra of the individual components of the mixture. Therefore, if the individual components are known, a channel-by-channel subtraction can be performed to strip out each contributor one at a time.

In spectrum stripping, the highest energy photopeak is selected, and its source is identified. A spectrum multiplier is determined by computing the ratio of the area of the sample photopeak to the photopeak area of a standard spectrum for that nuclide. This multiplier is then applied to each channel of the standard spectrum. The resulting spectrum is subtracted from the sample spectrum. The highest energy photopeak remaining is selected, and the process is repeated until all components are identified, stripped, and quantified.

Spectrum stripping is a reasonably accurate, but very tedious, procedure. Errors do creep into the results through the subtraction process because the shape of a standard spectrum can differ from that of a sample spectrum. Also, the error from counting statistics is propagated to the yet-to-be-stripped nuclides by the subtraction process. The principal reason for this shape difference is gain or threshold shifting of the photopeaks. Additionally, overlapping photopeaks can be a problem in both identification and quantification. For environmental work, photopeaks for radionuclides present at very low activity levels are difficult to identify.

A third method of analyzing gamma spectra is by simultaneous equations, which is very similar to methods used for simultaneous determinations of two or more components in spectrophotometric analysis. In this method, all nuclides in a sample must be identified, and each nuclide must possess an unobstructed photopeak. Again, this technique assumes that the contribution of each radionuclide to the sample spectrum is additive. The contribution of each radionuclide to the photopeak region of every other nuclide is determined from standard spectra. These are called interference factors. A set of simultaneous equations can then be written for all nuclides:

$$A_A = C_A + F_{BA} C_B + F_{CA} C_C + F_{DA} C_D + \ldots \quad , \qquad (3)$$

where A_A = counts in photopeak region of nuclide A,

C_A, C_B, etc. = counts due to nuclide A, B, etc.,

F_{BA}, F_{CA}, etc. = interference factors for nuclides B, C, etc., in the A photopeak region.

These simultaneous equations can then be solved by using matrix techniques to find C_A, C_B, etc.

The primary advantage of the simultaneous equations technique is its computer adaptability. The primary disadvantage is that the presence of an unidentified radionuclide in the sample invalidates all results. A large number of radionuclides cannot be handled without computer calculation. Also, complex, overlapping spectra are difficult to analyze, and the magnitude of errors increases with the number of nuclides in the sample. However, the error is very difficult to estimate at all.

The fourth method for resolving multicomponent gamma-ray spectra is linear regression analysis using the method of least squares. Least-squares analysis uses all data in all channels for estimating nuclide concentrations and can produce an error estimate for each nuclide concentration. In theory, this method produces the most accurate estimates for samples containing several nuclides.

4.7 LEAST-SQUARES ANALYSIS OF GAMMA-RAY SPECTRA

The resolution of a gamma spectrum into the concentrations of its component radionuclides can be treated as a curve-fitting problem by using least-squares techniques. The basic assumption is that the sample spectrum can be described by a linear combination of the gamma spectra of each component obtained separately. This discussion is intended to present the least-squares approach in nonmathematical terms.[4,5,11,12]

The linear least-squares method assumes that the pulse-height spectrum to be analyzed consists of the summed contributions of n nuclides, each of which is represented as a pulse-height spectrum of k channels. This method requires standard spectra, representing the response of the detector to gamma rays of the nuclides of interest, for comparison. The count rate in a sample spectrum due to standard j ($j=1...n$) in channel i ($i=1...k$) will be C_{ij}, and the total count rate in channel i will be X_i. The expression,

$$X_i = \left(C_{i1} + C_{i2} + C_{i3} + \cdots\right) = \sum_{j=1}^{n} C_{ij} \quad , \tag{4}$$

accounts for all contributions to channel i.

To obtain quantitative results from resolving a spectrum, the quantity of nuclide j must be expressed in terms of the standard for nuclide j. Therefore, a normalization factor M_j, the ratio of the activity of nuclide j in the unknown to the value of nuclide j in the standard, must be included:

$$X_i = \sum_{j=1}^{n} M_j S_{ij} + R_i \quad , \tag{5}$$

where R_i represents the random error in the channel i counts and S_{ij} is the count rate of the standard j in channel i. C_{ij} is simply the product of M_j, the normalization factor, and S_{ij}, the standard count rate.

If the only error in this calculation is the random error of the counts in a channel, R_i, then the least-squares technique can be used. This method estimates the parameters that minimize the weighted sum of the squared difference between two sets of values. The usual case has one set of values as observed data (X_i) and another set of computed values:

$$\left(\sum_{j=1}^{n} M_j S_{ij}\right) .$$

This translates to

$$\text{Minimize} \left(X_i - \sum_{j=1}^{n} M_m S_{ij} \right)^2 W_i \quad , \tag{6}$$

where W_i is the weighting factor chosen to estimate the variance of the counts in a channel. The use of weighting is important because it allows the more important spectral features, such as photopeaks, to be more highly emphasized in the calculation. If the variance is estimated for each channel, the result is a set of linear simultaneous equations (one for each nuclide of interest) that may be solved for the values of M_j. This solution is most easily derived by using matrix techniques on a computer.

Again, the least-squares method is theoretically the most accurate method for determining the activity of a composite sample. This technique uses all data in all channels to estimate the nuclide concentrations. In addition, the error in the calculation for each nuclide concentration is available from an intermediate step of the linear least-squares computation.[13] Once established, this type of computer program can be used to process large volumes of spectral data.

Disadvantages of the least-squares method are the initial adaptation of the computer program to available processing equipment and the initial evaluation of the computer program analytical results. Procedures for both operations are discussed in the following sections. Ill-conditioned equations, those equations whose solutions are sensitive to very small alterations in coefficient values, can cause the program to produce invalid results. Certain combinations of nuclides having similar spectral shapes or overlapping peaks can cause such a problem. These instances must be examined individually. These problems will be discussed further in Section 6.

In summary, a properly applied least-squares technique can yield superior results, as compared with any other method of analyzing NaI(Tℓ) complex gamma-ray spectra. However, the installation of such a computer program requires that the user be aware of the programming and statistical obligations that must be fulfilled to create useful and sound results.

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SECTION 5

ALPHA-M

5.1 GENERAL

The multicomponent gamma-ray spectrum analysis program ALPHA-M was developed by E. Schonfeld in 1965[1,2] and modified for this study by S. Seale (TVA) in 1975. ALPHA-M determines the activities of radioisotopes by a weighted least-squares resolution of their gamma-ray spectra. The application of the least-squares method to gamma spectral data yields superior quantitative results as compared with any other commonly used technique. There are several immediate advantages of this technique:

1. Rapid data processing is possible.

2. Spectra with large statistical variations in counting can be handled.

3. The total spectrum, rather than just the photopeak regions, is used.

4. Spectra with superimposed peaks can be analyzed.

5. The standard error of the nuclide activity can be estimated.

5.2 BASIC FEATURES

5.2.1 Library Standards

The 1975 version of ALPHA-M allows the input of up to 20 library standards of 256 channels each for one to four detectors. Simple modifications (see Appendix A) allow further expansion of the library. ALPHA-M can select for a particular analysis any combination of library members, as requested, ranging from a single radionuclide standard to a composite of all members of the library.

5.2.2 Background Compensation

ALPHA-M can accept samples whose background component has been subtracted in the multichannel analyzer. The program will convert meg complements (i.e., a number such as 999887) that arise from statistical counting variations to their correct negative values. ALPHA-M can also subtract a background spectrum from sample spectra. Background compensation may also be achieved by including the background as a library standard, and a background spectrum may be entered to replace the library background spectrum for special data processing. This last option does not change the actual stored standard library, but only the one being used by the program for the particular analysis.

5.2.3 Activity Corrections

The program can take into account corrections for counting time, decay time, analytical sample size, and concentration of the sample before analysis, thus allowing the user to receive corrected results in the desired units (e.g., pCi/ℓ, pCi/g).

5.2.4 Standard Error Estimates

ALPHA-M produces a standard error for each radionuclide determined in the least-squares process. The standard errors may be used to erect statistical confidence intervals or to test statistical hypotheses about the determined activities.

5.2.5 Weighting Schemes

Several weighting methods are available to the program user. Sample spectra can be weighted by the observed channel contents, calculated channel contents, unity, or variance of the observed or calculated channel contents.

Recommendations for routine weighting options are made in Section 6.

5.2.6 Gain and Threshold Shift Compensation

ALPHA-M is able to compensate automatically for the gain and threshold shifts that may occur during sample counting; both shifts are included as elements of the least-squares process.

5.2.7 Rejection Coefficient

If the concentration of a radionuclide (or radionuclides) is negative or less than a predetermined fraction of the standard error, ALPHA-M can repeat the entire analysis and omit the standards for the rejected radionuclides. This may improve the accuracy and sensitivity while reducing the standard errors of the remaining radionuclides.

5.2.8 Analyses of Residuals

The modified version of ALPHA-M includes a new option for allowing a more detailed analysis of the residuals obtained from the fitting process.[3-5] To describe the distribution of the standardized residuals, the program outputs the mean, standard deviation, skewness, and kurtosis of the residuals. The program also prints the percentage of the residuals within one, two, and three standard deviations of the residual mean. A plot of the normalized residuals vs. channel number can be requested. The program identifies as "suspicious" those channels lying outside a ±3 standard deviation band surrounding the residual mean.

5.2.9 Other Minor Features

A calculation of the coefficient of variance (or variation) has been added to ALPHA-M. This coefficient provides a measure of comparison of the relative precision of estimates whose magnitudes vary over a wide range. A program option has been added to calculate and print out the intervariable correlations after the terminal cycle of least-squares refinement. This correlation shows the degree to which any two variables are interrelated in the calculations.[6,7] The subroutine INVERT has been modified to execute in double precision.

5.2.10 Diagnostics Package

A series of diagnostics has been included to warn users of errors or possibly unwise combinations of option selections. In general, these diagnostics will stop sample processing and give a diagnostic message. However, certain diagnostics do not stop sample processing, but do provide a warning if data from a particular determination are questionable. For example, the matrix inversion subroutine has been rewritten to test for pivots smaller than 1.0×10^{-10} and to change them, if found, to 1.0. This "fixup" not only prevents the occurrence of a floating-point divide check, which would stop processing, but also prints the warning that a singular matrix has been encountered. This diagnostic informs the user that the results of the particular analysis are meaningless.

5.2.11 Alpha Factors

The alpha factor expresses the ratio of the variance of an estimate to the sum of the variances of all other variables in the determination. This quantity is roughly proportional to the weight of a specified variable in the determination. The alpha factors are independent of the sample spectrum and are descriptive of the standard nuclide library. Therefore, alpha factors can be used to monitor the quality of new sets of standards prepared for ALPHA-M.

5.2.12 Input/Output

The modified version of ALPHA-M has an entirely new input and output structure. All input instructions, input data, analytical results, and performance indicators are now clearly displayed and labeled on the resulting printouts.

5.2.13 Lower Level of Detection

This version of ALPHA-M also provides an estimate of the lower limit of detection (LLD) for a particular determination. This LLD value is calculated from the technique developed by Altshuler and Pasternack[8] and Pasternack and Harley[9] and is illustrated in HASL-300.[10]

5.3 STANDARDS AND DATA FOR ALPHA-M

The basic assumption of the least-squares approach to gamma-ray spectrum analysis is that the experimental conditions for the standard and sample spectra are identical. The most important consideration is the maintenance of a constant energy scale for all data collection, which requires a daily calibration procedure with a specified set of radionuclide sources. This calibration procedure must be duplicated exactly on every occasion to ensure constant spectrometer performance. In addition to this major daily calibration, the user should make fine gain adjustments between samples to account for intraday gain variations. This can be done by recentering the 662-keV peak of ^{137}Cs to the correct scale position by adjusting the amplifier fine gain between sample runs.

Another requirement for the standard library is that the variability in the library standards must be less than that in the sample spectra. For example, if a routine sample is expected to have an average activity of 100 disintegrations per minute (dpm), then the standards in the library should have activity levels of 1000 to 10,000 dpm. An alternative method is to use standards with lower activity levels and to count them for ten times as long as the samples will be counted. The latter approach avoids the problems of summing and gain shift due to high count rate; however, gain variations resulting from bias and temperature fluctuations do become important with longer count times.

If background spectra are to be used with ALPHA-M, they must be determined under conditions identical to those used for the library standards and sample spectra. Heavy shielding should be used for environmental work, to reduce fluctuations of background activity during sample analysis.

A program called GEN4 (Appendix B) may be used to generate the standard library spectra for ALPHA-M. The program assumes that the average user will store the standard libraries on a computer-accessible mass storage medium rather than read the standards from cards for each processing run.

The reference library may be constructed with up to 20 standard spectra (of 256 channels each) for one to four detector geometries. A standard background spectrum may be included in the library by submitting to the program a number of daily background spectra, which are then averaged. Reference spectra may be supplied to GEN4 with the sample background previously subtracted by the analyzer, or the standard background may be averaged by the program and subtracted from all input spectra. The library produced by GEN4 contains all data regarding names, half-lives, counting times, and activities of the standard nuclides.

Operating in the update mode, the program can replace any library standard spectrum and its identifying header. Because GEN4 assumes that such changes will be made to the background standard only, there is no provision to modify the appropriate information record (activity, name, half-life, etc.) for the specified standard. In other words, a library standard with an activity different from the original library member cannot be added to the library without recreating the entire library.

Printed output from GEN4 includes all information recorded on the information records as well as tabulated values for all standard spectra input. The sum of all channel counts for each library spectrum is also displayed.

Specific information for using GEN4 is included in Appendix B. All ALPHA-M code statements relating to input or storage of standards, or their use in calculations, have been restructured or rewritten to conform with the standards library created with GEN4. Both GEN4 and ALPHA-M can be easily modified to provide for completely different detector libraries; instructions for the changes that must be made are included in Appendix B.

5.4 ALPHA-M INPUT INSTRUCTIONS

Certain control cards are necessary to operate ALPHA-M. Table 1 lists each control variable, its position on the control or option card, and its correct format. Figure 4 illustrates the basic loop structure of ALPHA-M, and figure 5 shows the arrangement of the input card deck for ALPHA-M.

The general control card controls (1) the overall program input-output and (2) the computational limits that apply to all samples to be processed. The usual values for the general control card variables are

TABLE 1. ALPHA-M INPUT INSTRUCTIONS

(General Control Card - 11I4, 8A4)

Variable	Columns	Format	Description
M	1-4	I4	Number of channels in spectra.
NIT	5-8	I4	Maximum number of iterations in least-squares refinement process.
NBA	9-12	I4	1 = To print library standards. 0 = Not to print library standards.
NZ	13-16	I4	Initial channel for computation.
MF	17-20	I4	Final channel for computation.
NTS	21-24	I4	Fortran logical unit on which the standard nuclide library resides.
NTM	25-28	I4	Fortran logical unit on which the sample spectra and background reside.
MU	29-32	I4	Fortran logical unit for print-plots.
NH	33-36	I4	1 = To print correlation coefficients. 0 = Not to print coefficients.
IAUX	37-40	I4	If IAUX greater than zero, auxiliary data will be output on Fortran logical unit IAUX for further processing.
IOPT	41-44	I4	If IOPT greater than zero, analytical results will be output on Fortran logical unit IOPT for further processing.
FM	45-76	8A4	This is the format (enclosed in parentheses) under which all sample spectra and backgrounds will be read.

TABLE 1 (cont.)

(Sample Control Card - A8, 4I3, 5F9.4,
One Card Per Sample)

Variable	Columns	Format	Description
XIDT	1-8	A8	Eight character sample identification.
NOPT	9-11	I3	Number of processing options (also the number of option cards to read).
NBR	12-14	I3	0 = Do not read background for this sample. 1 = Read a background spectrum for this sample; also use this background for all subsequent samples until another is read in.
NBS	15-17	I3	1 = To subtract background permanently for this sample (applies to all processing options). 0 = Do not permanently subtract the background for this sample (the background may still be subtracted for specified options).
IABP	18-20	I3	1,2,3, or 4 for detector A,B,C. or D.
MS	21-23	I3	If greater than zero, the last background spectrum input will be exchanged with the nuclide standard MS for the purposes of computation. (Actual spectrum in library remains unchanged.) This change is permanent for duration of the job or until another substitution is made on a subsequent sample.
TB	24-32	F9.4	Counting time (in minutes) for background spectrum.
TSA	33-41	F9.4	Counting time (in minutes) for sample spectrum.
VRED	42-50	F9.4	Volume Reduction Factor (calculated sample activity is divided by this factor).

TABLE 1 (cont.)

(Sample Control Card, Cont.)

Variable	Columns	Format	Description
DAY	51-59	F9.4	Decay time in days between sample acquisition date and counting date.
VM	60-68	F9.4	Volume multiplication factor (calculated sample activity is multiplied by this factor).

(Background Spectrum Cards)

A set of cards or card images residing on the logical unit specified on the General Control Card and consisting of

1. A 20A4 identifying header card.
2. As many cards or images as required by the format specified on the Format Control Card.

(Sample Spectrum Cards)

A set of cards or card images residing on the logical unit specified on the General Control Card and consisting of

1. A 20A4 identifying header card.
2. As many cards or images as required by the format specified on the Format Control Card.

[Sample Option Card - 6I3,3F6.2(22I2), a Set of NOPT Cards]

Variable	Columns	Format	Description
N	1-3	I3	The number of standard nuclides to use from the library.
NB	4-6	I3	1 = To subtract background from sample for this processing option. 0 = Do not subtract the background.

TABLE 1 (cont.)

(Sample Option Card, Cont.)

Variable	Columns	Format	Description
NW	7-9	I3	1 = For weights based on reciprocal of the calculated counts/channel. 2 = For weights based on the reciprocal of the variance of the calculated counts/channel (requires that a sample background be present). 3 = For unit weights. -1 = For weights based on the reciprocal of the observed counts/channel. -2 = For weights based on the reciprocal of the variance of the observed counts/channel (requires background).
KT	10-12	I3	2 = For automatic gain and energy threshold shift compensation. 1 = For automatic gain shift compensation only. 0 = For no compensation. -1 = For manual compensation - requires input values of gain and threshold shifts on a card immediately following this option card. -2 = To base the values of gain and energy threshold shift on the results calculated from a previous sample (The value of QH on this card must be set to a negative value).
IRD	13-15	I3	0 = For no print-plots. 1 = For print-plots of residuals. 2 = For print-plots of residuals, calculated and observed spectrum.
IPRINT	16-18	I3	1 = To print matrices for each cycle. 0 = For no matrices for each cycle.
QH	19-24	F6.2	Energy offset, in channels or fractions of a channel, between the spectra in the standards library and the sample spectrum. Leave blank if unknown.

TABLE 1 (cont.)

(Sample Option Card, Cont.)

Variable	Columns	Format	Description
Q	25-30	F6.2	0 = For no rejection cycle. n.m = To apply a rejection ratio of n.m. (Refer to 5.4.)
XMOD	31-36	F6.2	Modifier for weighting scheme. (Refer to 5.4.)
IS(1)	37-38	I2	The numbers of the "N" library standards selected for analysis.
IS(2)	39-40	I2	
IS(3)	41-42	I2	
--	---	--	
IS(N)	---	--	

(Manual Shift Card - 2F10.4, This Card Required Only if KT = -1)

Variable	Columns	Format	Description
FTT	1-10	F10.4	Value of gain factor to apply.
SHCT	11-20	F10.4	Value (in channels) of the energy threshold shift to apply.

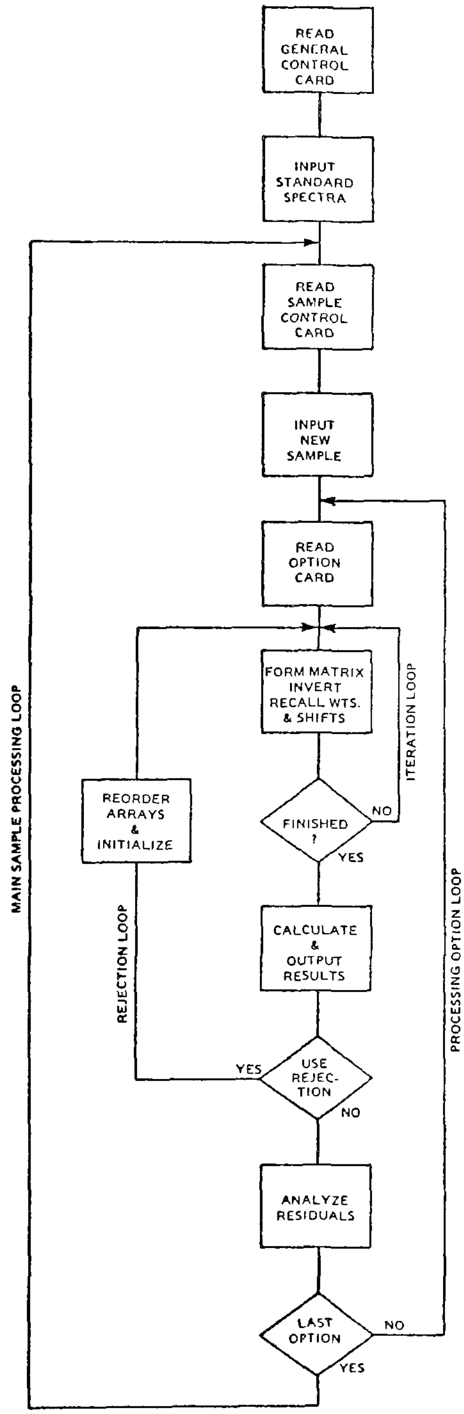

Figure 4. Basic loop structure of ALPHA-M.

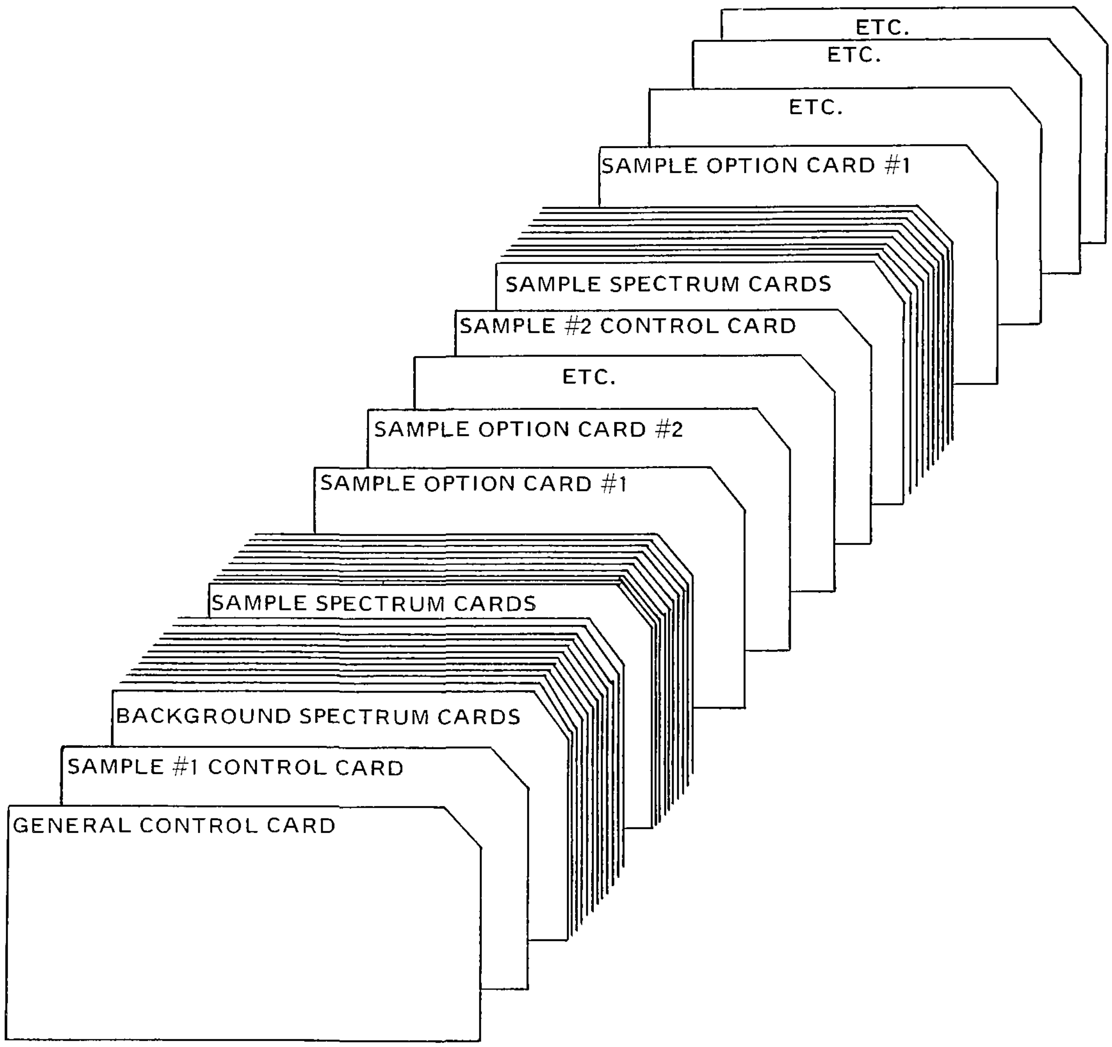

Figure 5. Arrangement of input card deck for the ALPHA-M program.

M	NIT	NBA	NZ	MF	NTS	NTM	MU	NH	IAUX	IOPT	FM
256	5	0	10	181	11	5	9	0	0	1	(10F7.0).

Since ALPHA-M is set up to use 256 channels of data, the parameter M never changes. Experience has shown that five iterations (NIT) are sufficient to resolve most spectra. ALPHA-M will terminate the run after less than five iterations if the chi-square per degree of freedom (CHDF) falls low enough (<1.2) or if the iterations are diverging rather than converging. The library standards (NBA) are not usually printed because of the large volume of print required. The selection of the initial channel (NZ) for calculations is arbitrary. Our laboratory selects channel 10 as the first calculation channel--the first nine analyzer channels are empty because pulse discrimination is used to remove the influence of the lead X rays and bremsstrahlung that arise at low energies. Our laboratory selects channel 181 as the final channel for computation (MF) because no radionuclide for which we are analyzing has a gamma ray with an energy above 1.7 MeV. This channel selection option saves CPU time in the calculations, but the limits will vary with the user. Correlations (NH) are not normally requested for routine operation because of the extra print requirements. All data entered into ALPHA-M by our laboratory are punched or stored in the same 10F7.0 format (FM). Other users may wish to change this format

The variables NTS, NTM, MU, IAUX, and IOPT all identify Fortran logical units from which or to which the program reads or writes information; they are defined by the system control cards required to execute the program. An example of this setup for an IBM system is given in Appendix A.

For routine processing, the optional printed outputs such as correlation coefficients, library standards, and residual plots are not requested because of the large amount of required print. If a sample analysis appears to be unsatisfactory, these options could be selected on a rerun of the sample to determine the source of the poor performance.

The next card in the control file is the sample control card. This card contains specific information used to properly identify and correct the final calculated activities for the particular sample being analyzed. For a 10-day-old, 3.5-liter water sample that was counted for 4000 seconds to yield a final answer in pCi/ℓ corrected to the actual time of collection, the sample control card might look like:

XIDT	NOPT	NBR	NBS	IABP	MS	TB	TSA	VRED	DAY	VM
TEST1	1	0	0	2	0	66.67	66.67	3.5	10.0	0 .

For routine processing, the preferred method of accounting for the background is to use a background library standard (Section 6). Therefore, no background is read by ALPHA-M unless overridden by this card using variable NBR (NBR > 0). To enter an individual background for a particular sample, the best method of processing (NBS) is to not subtract the background permanently. Of course, if only one processing option is to be run, permanent subtraction is permissible. However, once a background is permanently subtracted, the original sample spectrum cannot be restored for analysis by another processing option requiring the nonstripped spectrum.

If a "background read" is requested, the background data follows the sample control card in the control file. These data cards consist of a header card identifying the background followed by the background spectrum in the 10F7.0 format. The sample spectrum raw-data cards are the next cards of the control file read by ALPHA-M. These cards have the same arrangement and format as the preceding background data.

After the raw-data cards have been read, ALPHA-M reads the sample option card. ALPHA-M expects as many sample option cards as were specified by variable NOPT on the sample control card. A typical sample card has the following form:

N	NB	NW	KT	IRD	IPRINT	QH	Q	XMOD	IS(1)	IS(2)...
3	0	1	2	0	0	0	1.0	0	1	2...

ALPHA-M allows the user to specify how many and which nuclide standards to use for a particular processing option with the variables N and IS(1), IS(2), IS(3), etc. If the user is reasonably certain of which nuclides are present, those specific nuclides can be called. If the user does not have any information about the nuclides that are present, the entire library can be invoked. By using the rejection coefficient, Q, the program will make two passes on the data--the first using all requested nuclides and the second eliminating the library standards for those nuclides that had negative activities or error terms larger than the activity found. This rejection technique can achieve the same effect as using a reduced library. The use of the rejection coefficient is further discussed in Section 6. If rejection is not required, then a value of 0.0 is entered for variable Q.

The energy offset between library standards and the sample spectrum (QH) is very difficult to determine. Therefore, this variable should be left as zero except for test operations.

Data from this study and from Schonfeld's work[1,2] show that selection of automatic gain and threshold shift, KT=2, yields the most accurate results (see Section 6). Selection of the reciprocal of the calculated counts per channel, NW=1, appears to be the most stable weighting scheme. The various weighting options are also fully discussed in Section 6.

If IAUX on the general control card is set for greater than zero, the user can select which, if any, options to write out for residual analysis with the variable IRD on the sample option card. IPRINT allows examination of the calculation matrices for samples that yield poor results or that have received a singular matrix warning on a previous run.

It is strongly suggested that the user select a zero value for XMOD. All analyses in this report were performed for XMOD=0.0. Any suggested change should be made only after an extensive investigation of its effects on the refinement process. XMOD appears in the weighting expression $(Y + 1.5 + XMOD)^{-1}$ and therefore could have a marked effect on the analytical results.

If the variable KT on the sample option card has been set at -2, a manual shift card must follow the sample option card. The manual shift card tells ALPHA-M the values of gain and threshold shift to apply to the sample spectrum.

5.5 ALPHA-M OUTPUT

The output from ALPHA-M is shown in figure 6. The first page of output reflects the information received by ALPHA-M from the general control card. The information records for the library standards requested are also printed on this page, thus allowing the user to see that the proper standards were indeed selected.

Page two of the ALPHA-M output reflects the information on the sample control card. The sample number heading on this and following pages indicates the location of the sample in the stream of samples submitted for analysis. If a background spectrum is entered, it appears on page two before the sample spectrum. The sum of all observed channel counts is calculated and printed for both the background and sample spectra. This can serve as a check for bad data transmittal, if these values are determined in the analyzer before submittal to ALPHA-M.

The fourth page of output reflects the input information from the sample option card. The first results listed from the ALPHA-M calculations are the CHDF, threshold shift, and gain shift values for each iteration, followed by the

ALPHA-M VERSION 2 LEVEL 3 RADIOANALYTICAL LABORATORY DATE: 05/21/76 TIME:15:31:08

GENERAL CONTROL INFORMATION

DATA FORMAT IS (10F8.1)
NUMBER OF CHANNELS IN ANALYZER IS 256
MAXIMUM NUMBER OF ITERATIONS IS 5
INITIAL CHANNEL FOR COMPUTATION IS 10
FINAL CHANNEL FOR COMPUTATION IS 181
STANDARD SPECTRA ON FORTRAN LOGICAL UNIT 3
SAMPLE SPECTRA ON FORTRAN LOGICAL UNIT 5
LIBRARY STANDARD SPECTRA WILL NOT BE PRINTED
CORRELATIONS BETWEEN VARIABLES WILL BE PRINTED
AUXILIARY DATA OUTPUT ON FORTRAN LOGICAL UNIT 4
ANALYTICAL RESULTS OUTPUT ON FORTRAN LOGICAL UNIT 2
FORTRAN LOGICAL UNIT FOR PRINT-PLOTS (IF REQUESTED) IS 9

FILE CONTAINS DATA FOR GEOMETRY TYPE 3.5L WATER NUMBER OF STDS IS 15 NUMBER OF DETECTORS IS 4

NUCLIDE	HALF-LIFE(DAYS)	CNT-TIME(MINS)	ACT-DET-A	ACT-DET-B	ACT-DET-C	ACT-DET-D
BACKGRND	**********	66.66667	350.0	350.0	350.0	350.0
144CE-PR	285.0	66.66667	3217.0	3217.0	3217.0	3217.0
51CR	27.7	66.66667	4903.0	4903.0	4903.0	4903.0
131I	8.1	66.66667	4525.0	4525.0	4452.0	4452.0
106RU	369.0	66.66667	4151.0	4151.0	4151.0	4151.0
134CS	767.0	66.66667	6941.0	6941.0	6941.0	6941.0
137CS	11100.0	66.66667	3803.0	3803.0	3803.0	3803.0
95ZR-NB	65.0	66.66667	14540.0	14540.0	14540.0	14540.0
58CO	70.8	66.66667	7193.0	7193.0	7264.0	7264.0
54MN	313.0	66.66667	6318.0	6318.0	6318.0	6318.0
65ZN	245.0	66.66667	2538.0	2538.0	2538.0	2538.0
60CO	1920.0	66.66667	4630.0	4630.0	4630.0	4630.0
40K	**********	66.66667	22250.0	22250.0	22293.0	22250.0
140BA-LA	12.8	66.66667	5950.0	5933.0	6011.0	5994.0
RADON	**********	66.66667	350.0	350.0	350.0	350.0

Figure 6. ALPHA-M output.

CONTROL INFORMATION ..... SAMPLE NUMBER 1   SAMPLE ID IS: I-131-50

NUMBER OF PROCESSING OPTIONS IS 1
COUNTING TIME (MINS.) FOR BKGND IS 66.67
COUNTING TIME (MINS.) FOR SAMPLE IS 66.67
DECAY TIME (DAYS) IS 0.0
VOLUME REDUCTION FACTOR IS 3.500
VOLUME MULTIPLICATION FACTOR IS 1.000
SAMPLE TIME/BKGND TIME = FS = 1.000
VALUE OF FS**2 = FX = 1.000
SAMPLE BACKGROUND WILL BE INPUT AND USED IF SUBTRACTION REQUESTED
PERMANENT BACKGROUND SUBTRACTION NOT REQUESTED
DETECTOR A STANDARDS SELECTED

TEST BACKGROUND IS LIBRARY STANDARD NUMBER ONE

4000.0	0.0	0.0	0.0	0.0	0.0	190.9	638.1	751.2	777.5
719.2	675.6	704.7	732.6	779.0	781.6	773.7	748.9	728.0	736.0
705.2	702.2	668.0	706.5	713.2	664.8	614.0	581.2	583.4	579.1
555.1	516.9	495.5	491.4	510.3	534.9	494.9	435.2	387.6	358.0
337.9	332.8	333.9	311.5	309.7	316.2	324.7	329.8	333.2	343.4
350.7	353.1	317.1	290.4	276.8	244.9	249.1	259.5	254.7	272.9
265.9	267.1	244.0	221.2	206.0	197.6	178.0	179.9	179.8	175.1
174.5	164.7	161.2	168.1	151.8	158.8	157.1	148.4	152.4	155.3
146.7	141.7	141.2	142.3	136.7	134.2	138.1	135.0	132.8	124.9
124.7	124.1	125.1	128.5	114.7	112.3	112.5	115.2	109.5	110.5
110.7	105.8	103.6	105.1	106.6	102.5	104.8	106.1	110.8	108.7
107.6	99.8	101.3	91.2	93.9	91.1	87.6	87.3	82.8	86.8
83.2	80.0	79.9	72.0	79.9	70.3	72.6	75.9	70.3	76.6
74.6	74.8	80.3	80.1	90.3	93.6	98.3	95.3	99.6	93.4
94.9	93.9	85.9	75.4	73.3	64.9	57.5	52.7	51.5	48.9
46.2	48.2	45.7	45.3	46.9	45.0	42.7	45.8	44.3	45.6
45.3	46.2	45.3	48.5	49.9	48.3	51.7	53.0	56.3	49.6
50.7	47.4	45.9	45.0	39.3	35.7	31.5	37.4	31.3	32.5
28.5	27.6	31.2	26.0	32.1	23.3	26.9	27.8	24.0	26.9
25.6	24.1	25.4	24.7	23.7	24.0	22.9	24.8	25.8	24.3
23.8	26.6	25.8	26.8	27.8	30.1	26.3	27.9	28.7	31.5
32.1	31.8	28.3	27.3	28.4	27.8	26.6	25.8	23.4	20.7
22.5	19.2	17.9	17.5	17.4	17.2	17.5	16.8	15.3	17.7
16.8	16.7	17.1	16.6	16.3	16.8	15.8	16.7	17.2	17.7
18.4	16.3	18.8	7.3	0.2	0.1	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0				

Figure 6. ALPHA-M output (cont.)

SAMPLE CONSISTS OF 50 PCI/LITER I-131 + BACKGROUND

1.0	0.0	0.0	0.0	0.0	0.0	178.2	667.3	772.9	853.1
792.7	669.5	781.8	771.4	791.8	916.0	945.2	916.8	789.2	845.0
896.3	739.8	699.6	791.4	695.1	713.5	709.7	634.6	596.3	669.0
602.0	554.2	527.6	524.3	693.7	676.0	829.6	798.8	605.6	480.2
392.3	357.3	293.7	304.7	332.7	309.7	297.4	368.3	331.6	346.1
335.2	356.2	299.1	314.9	300.7	236.8	297.4	229.7	253.4	304.7
262.1	320.6	268.2	207.6	252.8	207.6	190.8	171.3	170.8	166.9
174.8	171.2	170.4	189.1	142.0	125.0	140.0	141.7	137.3	138.9
112.2	117.6	134.8	146.0	120.8	150.0	129.8	160.2	118.9	144.5
137.8	134.5	123.5	143.0	106.1	88.5	128.8	101.1	107.9	108.5
107.8	121.1	86.7	104.9	122.9	103.3	127.1	117.2	90.0	95.0
99.1	93.7	105.7	79.2	95.1	101.6	78.6	78.2	94.3	93.9
96.5	81.7	63.6	75.3	61.4	53.3	65.8	89.6	71.2	59.3
77.0	86.3	71.5	81.4	76.1	88.2	86.8	91.2	107.1	92.4
103.1	87.0	62.5	63.4	76.4	57.0	59.6	48.1	62.3	77.2
43.6	52.2	62.8	45.7	53.1	39.0	39.6	40.8	60.1	51.9
38.6	37.8	32.0	58.3	53.6	52.8	46.2	41.3	52.4	54.7
56.1	54.7	40.0	41.8	45.6	33.2	40.0	22.6	36.0	26.0
36.8	24.0	27.0	20.8	22.4	27.6	30.6	27.6	28.1	33.5
19.0	20.9	22.8	35.6	34.2	18.5	27.8	27.9	26.1	30.1
24.6	20.9	21.1	32.5	42.1	33.7	26.8	31.1	27.7	36.0
25.8	38.0	31.5	26.2	34.1	38.6	20.2	26.0	27.8	33.4
9.7	15.5	7.5	12.0	14.8	14.1	13.4	20.9	22.2	13.5
11.1	18.6	9.5	20.3	18.2	19.4	5.5	17.8	14.0	9.0
17.7	9.6	18.7	6.9	1.5	-1.1	0.3	-2.0	2.5	-0.7
2.1	1.8	0.8	0.4	0.2	0.7				

BACKGD SUM= 37563. SAMPLE SUM= 40698.

Figure 6. ALPHA-M output (cont.)

```
SAMPLE NUMBER  1     ID NO. I-131-50 ... PROCESSING OPTION NUMBER  1


BACKGROUND WILL NOT BE SUBTRACTED THIS OPTION
WEIGHTS TO BE BASED ON CALCULATED SAMPLE SPECTRUM
WEIGHTS PROPORTIONAL TO RECIPROCAL COUNTS/CHANNEL
REJECTION COEFFICIENT OF   1.00 WILL BE APPLIED
AUTOMATIC COMPENSATION REQUIRED FOR GAIN AND THRESHOLD SHIFT
NUMBER OF ISOTOPES USED FROM LIBRARY IS 15
THRESHOLD CHANNEL SHIFT BETWEEN STDS AND SAMPLE IS  0.0
LIBRARY STD. NUMBERS, IN ORDER OF DESIRED OUTPUT ARE  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15
NORMALIZED RESIDUALS WILL BE PLOTTED
OBSERVED AND CALCULATED SPECTRA WILL BE PLOTTED
MATRIX INFORMATION WILL NOT BE PRINTED


CHDF =   0.97   THR SHIFT =  0.0568   GAIN SHIFT =  0.9996
CHDF =   0.90   THR SHIFT =  0.0991   GAIN SHIFT =  0.9991
CHDF =   0.86   THR SHIFT =  0.1196   GAIN SHIFT =  0.9988
CHDF =   0.83   THR SHIFT =  0.1309   GAIN SHIFT =  0.9986
CHDF =   0.82   THR SHIFT =  0.1384   GAIN SHIFT =  0.9985
```

CORRELATIONS

1	1.000															
2	-0.191	1.000														
3	0.036	0.016	1.000													
4	0.055	-0.025	-0.001	1.000												
5	-0.291	-0.072	-0.041	0.013	1.000											
6	0.044	0.148	0.203	0.341	-0.102	1.000										
7	-0.314	0.026	-0.029	-0.004	-0.082	-0.049	1.000									
8	-0.291	-0.025	-0.063	-0.057	0.236	-0.276	0.049	1.000								
9	0.052	-0.051	-0.087	-0.182	-0.265	-0.468	0.070	-0.283	1.000							
10	-0.150	0.018	0.027	0.050	0.334	0.096	-0.032	0.338	-0.794	1.000						
11	-0.127	0.083	0.057	0.134	-0.056	0.113	0.044	-0.012	-0.059	-0.007	1.000					
12	-0.437	0.151	0.090	0.135	0.176	0.065	0.125	0.077	-0.077	0.084	-0.187	1.000				
13	-0.592	0.095	-0.004	0.032	0.203	-0.026	0.200	0.179	-0.032	0.085	0.035	0.141	1.000			
14	-0.631	0.131	-0.104	0.056	-0.081	0.128	0.229	0.120	-0.179	0.062	0.105	0.163	0.327	1.000		
15	-0.529	-0.092	-0.350	-0.557	0.051	-0.546	0.092	0.198	0.291	-0.049	-0.136	0.031	0.213	0.182	1.000	
16	0.126	-0.175	-0.031	0.207	0.065	0.057	-0.022	-0.024	-0.037	0.032	-0.015	0.017	-0.143	-0.116	-0.138	1.000
17	-0.172	0.246	0.109	-0.317	-0.067	-0.071	-0.040	0.008	0.032	-0.001	-0.002	0.011	0.114	0.116	0.192	-0.822

Figure 6. ALPHA-M output (cont.)

LIBRARY NUMBER	NUCLIDE NAME	DECAY UNCORRECTED ACTIVITY	DECAY UNCORRECTED STD. ERR.	DECAY CORRECTED ACTIVITY	DECAY CORRECTED STD. ERR.	COEFFICIENT OF VARIANCE	ALPHA FACTOR	LLD
1	BACKGRND	99.2208	3.6255	99.2208	3.6255	3.65	5.1268	11.9278
2	144CE-PR	-29.4729	12.7227	-29.4729	12.7227	43.17	0.5990	41.8578
3	51CR	-16.1977	24.5637	-16.1977	24.5637	151.65	0.9160	80.8147
4	131I	55.7074	4.4788	55.7074	4.4788	8.04	1.1009	14.7352
5	106RU	8.3461	12.8111	8.3461	12.8111	153.50	1.3733	42.1486
6	134CS	2.5162	4.1426	2.5162	4.1426	164.64	1.6750	13.6292
7	137CS	-0.2911	2.9736	-0.2911	2.9736	******	0.6184	9.7831
8	95ZR-NB	-1.7011	3.2002	-1.7011	3.2002	188.12	0.7197	10.5286
9	58CO	-14.4353	6.2361	-14.4353	6.2361	43.20	1.6821	20.5167
10	54MN	3.9251	4.7604	3.9251	4.7604	121.28	1.0588	15.6618
11	65ZN	-1.2014	5.9745	-1.2014	5.9745	497.28	0.8121	19.6562
12	60CO	-1.5538	2.6811	-1.5538	2.6811	172.55	1.0776	8.8207
13	40K	-46.5003	39.3006	-46.5003	39.3006	84.52	0.8725	129.2989
14	140BA-LA	5.0339	3.2990	5.0339	3.2990	65.53	1.9222	10.8536
15	RADON	2.6242	4.5061	2.6242	4.5061	171.72	3.4124	14.8252

NORMALIZED RESIDUALS PER CHANNEL

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.9	-1.4	-0.3	-0.5	-0.3	1.3	1.3	1.0	-1.3	-0.1
2.4	-0.7	-0.8	0.4	-1.7	-0.0	1.2	0.3	-1.5	0.2	-0.6	-0.4	-0.3	-0.6	2.1	-1.7	0.4	0.7	-1.1	0.2
0.9	0.7	-1.5	-0.3	0.7	-0.3	-1.2	1.2	-0.1	-0.2	-0.7	0.1	-0.5	1.0	1.0	-0.3	1.7	-1.4	-0.5	0.6
-1.0	1.0	0.0	-1.6	1.2	0.0	0.5	-0.5	-0.4	-0.4	0.1	0.5	0.7	1.2	-0.2	-1.4	-0.4	0.5	0.3	0.4
-0.6	-0.3	0.3	0.4	-0.9	0.8	-0.6	1.4	-0.8	1.2	0.9	0.6	-0.1	0.9	-0.3	-1.5	1.2	-0.8	-0.1	-0.1
-0.2	1.1	-1.1	0.1	1.1	0.1	1.6	0.7	-1.3	-0.8	-0.5	-0.3	0.3	-0.7	0.3	0.9	-0.5	-0.5	0.9	0.6
1.2	0.1	-1.3	0.2	-1.5	-1.3	-0.4	1.2	0.2	-1.2	0.4	1.0	-0.6	0.2	-0.8	-0.3	-0.7	0.1	0.8	0.3
1.0	-0.2	-1.3	-0.6	0.4	-0.4	0.2	-0.4	1.1	2.2	-0.5	0.1	1.0	-0.4	-0.1	-1.2	-0.8	-0.8	1.2	0.4
-0.9	-1.0	-1.2	0.9	0.3	0.3	-0.7	-1.2	-0.3	0.4	0.3	0.5	-0.7	-0.5	0.5	-0.3	0.7	-1.6	0.4	-0.7
0.8																			

AVERAGE =-0.0076 STD. DEV. = 0.8610 SKEWNESS = 0.1509 KURTOSIS = 2.5276
PERCENT OF RESIDUALS UNDER 1 SIGMA = 65.1 2 SIGMA = 97.1 3 SIGMA =100.0

SAMPLE/OPTION WRITTEN TO IOPT AT 05/21/76 15:31:18

Figure 6. ALPHA-M output (cont.)

```
SAMPLE NUMBER  1     ID NO. I-131-50 ... PROCESSING OPTION NUMBER  1

BACKGROUND WILL NOT BE SUBTRACTED THIS OPTION
WEIGHTS TO BE BASED ON CALCULATED SAMPLE SPECTRUM
WEIGHTS PROPORTIONAL TO RECIPROCAL COUNTS/CHANNEL
REJECTION COEFFICIENT OF   1.00 HAS BEEN APPLIED
AUTOMATIC COMPENSATION REQUIRED FOR GAIN AND THRESHOLD SHIFT
NUMBER OF ISOTOPES USED FROM LIBRARY IS  3
THRESHOLD CHANNEL SHIFT BETWEEN STDS AND SAMPLE IS  0.0
LIBRARY STD. NUMBERS, IN ORDER OF DESIRED OUTPUT ARE  1  4 14
NORMALIZED RESIDUALS WILL BE PLOTTED
OBSERVED AND CALCULATED SPECTRA WILL BE PLOTTED
MATRIX INFORMATION WILL NOT BE PRINTED

CHDF =   1.01   THR SHIFT =  0.0155   GAIN SHIFT =  1.0000
CHDF =   0.96   THR SHIFT =  0.0290   GAIN SHIFT =  0.9999
CHDF =   0.95   THR SHIFT =  0.0358   GAIN SHIFT =  0.9997
CHDF =   0.94   THR SHIFT =  0.0395   GAIN SHIFT =  0.9997
CHDF =   0.93   THR SHIFT =  0.0420   GAIN SHIFT =  0.9996

CORRELATIONS

  1   1.000
  2  -0.425   1.000
  3  -0.816   0.120   1.000
  4  -0.006   0.140  -0.043   1.000
  5  -0.031  -0.211   0.055  -0.811   1.000

 LIBRARY   NUCLIDE       DECAY UNCORRECTED          DECAY CORRECTED        COEFFICIENT    ALPHA
 NUMBER    NAME        ACTIVITY    STD. ERR.     ACTIVITY    STD. ERR.    OF VARIANCE    FACTOR       LLD
    1      BACKGRND     96.9487      1.5517      96.9487      1.5517          1.60       1.9363       5.1051
    4      131I         57.3890      3.5928      57.3890      3.5928          6.26       0.7793      11.8203
   14      140BA-LA      3.6308      2.8904       3.6308      2.8904         79.61       1.4861       9.5094

NORMALIZED RESIDUALS PER CHANNEL
   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.2   0.3  -2.0  -0.3  -1.2  -1.7   0.9   1.4   1.2  -1.3   0.2
   2.7  -0.9  -0.8   0.7  -1.7   0.1   1.3   0.3  -1.4   0.4  -0.4  -0.4  -0.5  -0.7   2.5  -1.4   0.9   0.7  -1.4   0.0
   0.8   0.8  -1.5  -0.3   0.9  -0.2  -1.1   1.4  -0.1  -0.1  -0.7   0.0  -0.7   0.9   1.0  -0.3   2.2  -1.2  -0.0   1.3
  -0.3   1.9   0.6  -1.2   1.6   0.1   0.5  -0.5  -0.4  -0.4   0.3   0.4   0.5   1.1  -0.6  -1.7  -0.9  -0.4  -0.8  -0.9
  -2.0  -1.5  -0.4   0.2  -0.9   1.0  -0.4   1.6  -0.7   1.3   0.9   0.8   0.0   1.0  -0.3  -1.4   1.2  -0.7   0.0   0.0
  -0.0   1.2  -1.0   0.1   1.3   0.2   1.6   0.9  -1.2  -0.8  -0.4  -0.3   0.4  -0.7   0.2   0.9  -0.5  -0.5   1.0   0.6
   1.3   0.2  -1.1   0.2  -1.3  -1.4  -0.4   1.2   0.2  -1.2   0.3   1.0  -0.6   0.2  -0.9  -0.3  -0.7  -0.1   0.6   0.1
   0.7  -0.4  -1.5  -0.8   0.3  -0.5   0.2  -0.4   1.1   2.6  -0.3   0.3   1.4  -0.2   0.2  -0.9  -0.6  -0.7   1.5   0.6
  -0.7  -0.9  -1.2   1.0   0.5   0.5  -0.5  -1.0  -0.2   0.6   0.6   0.8  -0.5  -0.2   0.7  -0.2   1.0  -1.5   0.6  -0.6
   1.1

AVERAGE = 0.0129           STD. DEV. = 0.9547          SKEWNESS =   0.3874        KURTOSIS =   2.6775
PERCENT OF RESIDUALS UNDER 1 SIGMA = 66.9     2 SIGMA = 95.9     3 SIGMA =100.0

SAMPLE/OPTION WRITTEN TO IOPT AT 05/21/76 15:31:22

* * * * * * * ALPHA-M NORMAL TERMINATION * * * * * * *
```

Figure 6. ALPHA-M output (cont.)

correlation coefficients. The values of the correlation coefficients reflect the interactions of the nuclides in the matrix inversion calculations. This correlation table is read by the row-column method used for determinants. The correlation between nuclides 6 and 10 is given in row 10, column 6. Correlation values consistently greater than 0.6 indicate that the two nuclides in question may interfere with each other in the analysis and therefore may weaken the least-squares model used by ALPHA-M. A discussion of this problem and possible solutions are included in Section 6.

The next results printed are the actual analytical results determined by ALPHA-M. The library number of the particular nuclide is written in the first column and the nuclide name is written in column 2. The two columns designated as DECAY UNCORRECTED contain the nuclide activity and standard error not corrected for decay. This uncorrected activity value is important for those radionuclides having short half-lives. If a sample was collected more than four half-lives before analysis, the uncorrected activity may show a value below the lower limit of detection for that nuclide. In such a case, the uncorrected activity value will indicate that the large results created by decay corrections are meaningless. In addition, the DECAY UNCORRECTED results should always be used in any statistical evaluation of program performance. This situation also is reflected in the LLD values found in the last column of results; these LLD values are corrected for decay.

The next double column is labeled DECAY CORRECTED and contains those nuclide activities and standard errors which have been corrected for decay. The coefficient of variance for a particular nuclide appears in column 5. This quantity is calculated by dividing the standard error of a particular nuclide by its calculated activity and multiplying by 100; this quantity will reflect the relative precision of the analysis.

After the analytical results, ALPHA-M prints out the standardized residuals. These residuals are the channel-by-channel difference between the observed and calculated values divided by the Poisson standard deviation of the observed value for a specified channel.[5] ALPHA-M provides some descriptive statistics for these residuals. The average value of the residual should be zero in the ideal case and close to zero in all cases. The standard deviation should approximate the CHDF value, and the skewness should fall between -0.464 and +0.464 for 150 data points. The value of kurtosis should range between 3.65 and 2.45 for 150 data points. The suspicious channels tabulated at the end of the printout are those channels lying outside a three-standard-deviation band surrounding the residual mean. These suspicious channels should be observed closely over a period of time to test the frequency with which certain channels appear. The recurrence of particular channels could indicate the presence of a nuclide in the samples for which there is no standard in the library.

For the printout in figure 6, ALPHA-M was requested to apply a rejection coefficient of 1.0 to the analysis results obtained by using the full set of library standards. Those library members selected for the second pass had contributions with standard errors that were smaller than the calculated activity on the first pass. The output for the second pass follows the same format as the first. The data from this second analysis should be an improvement in the analytical results for those nuclides used for the second determination since the number of library members is reduced. However, some very imprecise but real measurements may be rejected by this process. This is discussed more fully in Section 6.

5.6 REFERENCES

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SECTION 6

EVALUATION OF ALPHA-M

6.1 GENERAL

The performance of ALPHA-M depends on the properties of the standard spectra, the properties of the sample spectra, and the program processing options chosen. Summarizing this performance and resolving anomalous results during initial program installation and later operation require both some radiochemical and statistical expertise.

This section provides results to guide ALPHA-M users in their selection of program processing options. Methods also are presented for examining the standard libraries to determine their performance capabilities and for monitoring actual analytical results to test for anomalous values.

6.2 PROGRAM PROCESSING OPTIONS

ALPHA-M offers a large variety of options for sample analysis. The following decisions must be made before processing:

1. Whether background is to be (a) stripped (either by the analyzer or the program) from sample spectra or (b) included as a library standard.

2. Whether (a) both gain and threshold shift, (b) gain shift alone, or (c) no shift is to be applied to the sample spectra.

3. Whether the weighting scheme to be applied in the refinement process should be (a) reciprocal of the observed counts, Y_0^{-1}, (b) reciprocal of the calculated counts, Y_C^{-1}, (c) reciprocal of the observed counts plus background, DY_0^{-1}, (d) reciprocal of the calculated counts plus background, DY_C^{-1}, or (e) unity weights.

These choices lead to 30 different methods for analyzing sample spectra. The number of options can be reduced by eliminating the obviously poorer and theoretically unsound weighting schemes. Theory suggests that the weights should equal the reciprocals of the variances of the data being fitted.[1]

All weights based on observed counts should be disregarded for environmental work because of the large relative variability of counting statistics at low counting rates.

Also, unity weights should not be selected because unity in no way represents the variance of the data being fitted. Elimination of these weighting schemes reduces the possible processing options to 12.

If the sample spectra are stripped of background, simple weighting by Y_c^{-1} does not properly estimate the variance of the data points. Similarly, using DY_c^{-1} without stripping adds an extra background to the weights so that again the theoretical variance is not estimated.

Therefore, we are left with the choice of using (1) background stripping and the DY_c^{-1} weighting scheme or (2) background as a library standard and the Y_c^{-1} weighting scheme. These options are the only two weighting schemes that are compatible with theory. Of course, the shifting options have not been considered. To determine superiority among the remaining options, the program SIMSPEC (Appendix C) was used to simulate sample spectra for each of 12 different nuclides. Six spectra were created for each nuclide at an activity level of 50 pCi/ℓ and were analyzed using the remaining options. The average absolute percent error for each nuclide appears in table 2. These values are all somewhat high because the variances of the simulated spectra are not equal to the mean counts, but rather to twice the mean counts.

There is little difference between the two weighting options. However, in 9 of 12 cases, compensating for background by using a library standard gave a slightly smaller error. Treating the background as a library standard has the advantage that overall changes in background level are better compensated for in the processing.

Gain shifting is generally defined as the situation in which the energy zero intercept remains unchanged while the rest of the spectrum channel contents are shifted up or down in energy in a multiplicative fashion. Threshold shifting, however, is the translation of the entire spectrum along the energy axis in an additive fashion. For NaI scintillation spectra, normal gain shifts are usually cited as being less than 3 percent and threshold shifts are usually less than 1.5 channels. Note that the factors known as gain and threshold shifts are often merely components of a single effect produced by the variability of the detector-electronics package.

The gain and threshold shift procedure in ALPHA-M is based on an estimate of the derivative of the true spectrum obtained by differencing the observed spectrum.[2] This estimate, scaled in two different ways, is used to create two additional independent variables in the regression

TABLE 2. AVERAGE PERCENT ERROR WITH DIFFERENT PROCESSING OPTIONS[a]

Option	Nuclide (50 pCi/ℓ)											
	^{144}Ce	^{51}Cr	^{131}I	^{106}Ru	^{58}Co	^{134}Cs	^{137}Cs	^{95}Zr	^{54}Mn	^{65}Zn	^{60}Co	^{140}Ba
Strip DY_C^{-1} Gain-threshold shift	17.5	24.7	7.5	30.7	17.4	6.3	4.1	12.8	6.3	7.6	5.3	10.4
Strip DY_C^{-1} Gain shift only	27.4	33.4	7.1	28.8	19.2	6.2	4.3	12.7	3.6	6.9	5.3	10.4
Library BKG Y_C^{-1} Gain-threshold shift	15.7	31.6	6.4	24.8	14.6	6.5	5.7	11.9	5.0	6.9	5.8	11.3
Library BKG Y_C^{-1} Gain shift only	24.2	28.5	7.1	27.9	14.4	6.7	5.3	11.3	3.2	6.8	6.1	10.6

[a] $\%Error = \left| \frac{Known-Found}{Known} \right| \times 100$

equation. Because this estimate is subject to the counting fluctuations in the observed spectrum, these new independent variables may not match the effects of the gain and threshold shift very well.

Schonfeld tested the gain and threshold shift algorithms. on samples having activities well above environmental levels and showed that dramatic improvements in analytical results were obtained. Samples with environmental levels of activity were not tested.

Before evaluating any translational effect, such as threshold shifting in environmental spectra, one must determine the degree of accuracy with which the position of any peak can be determined. For a photopeak such as the 795.8-keV peak of ^{134}Cs (see the standards library in Appendix D), one may apply a least-squares Gaussian fitting process using the channel numbers and contents describing the peak to determine its position quite accurately.[3]

If (1) the contents of the photopeak channel and the contents of the two or three channels immediately below it are reduced by twice the square root of their contents, (2) the contents of the two or three channels above the photopeak are increased similarly, and (3) these values are then refit to a Gaussian, the exact position of the peak is shifted upfield by a small amount. If the process is reversed, the photopeak will be shifted downfield by a small amount. Thus, a small uncertainty in the position of any peak will exist because of counting statistics alone. This effect will be much more pronounced at environmental levels of activity than at levels such as those used by Schonfeld because the peaks are not as well defined.[1]

Table 3 illustrates the peak position error obtained by the above process for various photopeaks in the standards library. The average positional error is quite small (about 0.24 channel), but the errors range from 0.09 to 0.47 channel. Obviously, any threshold shift less than 0.50 channel will be difficult to detect.

If the channel and energy data in table 3 are fitted to a straight line, the estimated gain is 11.32 keV per channel. The energy error associated with the photopeaks in table 3 is shown in figure 7. Arguments similar to the above may be used to indicate that system gain is uncertain to a degree roughly equal to the expected gain shifts.

Shifts due to counting statistics or detector-electronics effects do occur, and thus the question of whether ALPHA-M can compensate for these shifts must be considered. To determine this, sample spectra consisting of a standard background plus nine nuclides, each at an activity level of

TABLE 3. PHOTOPEAK POSITIONS, ERRORS, AND ENERGIES

Nuclide	Energy (keV)	Peak Channel	Error Range (Chnls)
^{106}Ru	511.8	53.15	0.15
	622.1	63.35	0.32
^{58}Co	511.0	52.89	0.33
	810.6	80.09	0.24
^{134}Cs	604.7	61.25	0.19
	795.8	77.74	0.29
^{60}Co	1173.0	112.22	0.32
	1332.0	125.92	0.47
^{140}Ba	487.0	50.94	0.09
	815.8	80.81	0.23
	1596.0	148.20	0.25
^{40}K	1460.8	136.25	0.44
^{65}Zn	1115.5	107.02	0.27
^{54}Mn	834.8	82.49	0.15
^{95}Zr	756.7	75.69	0.18
^{137}Cs	661.6	66.88	0.11
^{51}Cr	320.1	34.34	0.13
^{131}I	364.5	38.90	0.12

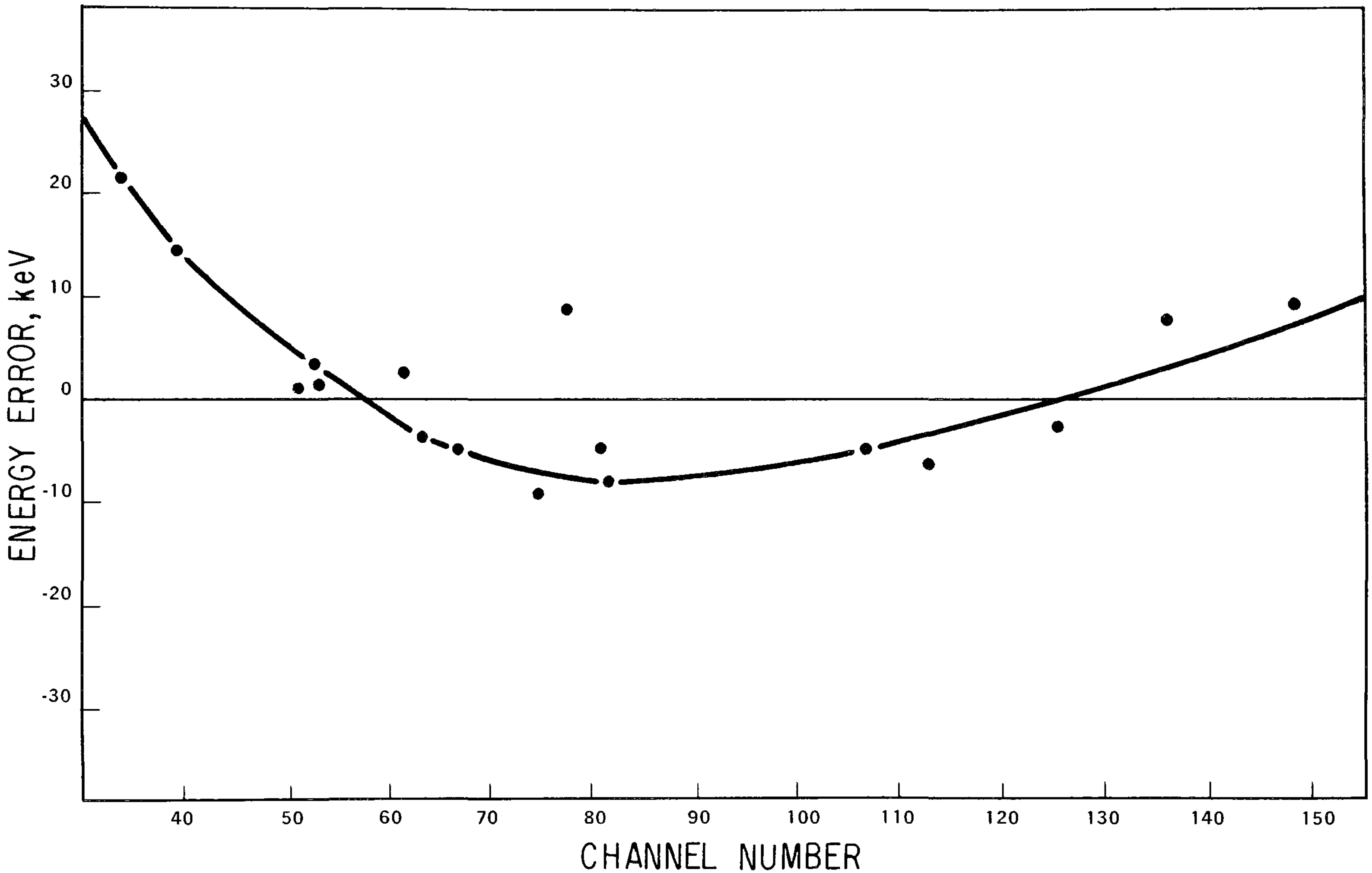


Figure 7. Energy error vs. photopeak position.

10 pCi/ℓ, were generated and randomized six separate times using SIMSPEC. The replicates were subjected to an ALPHA-M analysis with no shifting, after being shifted upfield by 1.5 percent and then after being shifted downfield by 1.5 percent. The results are shown in table 4. Because of the very high percent error at this low activity level and because of the number of components, any systematic effects are hopelessly masked. However, a gain shift of 1.5 percent, which corresponds to a positional shift of about 1.0 channel for the ^{137}Cs standard, does not move the average percent error outside the range observed with no shift.

Most threshold and gain shifts, as reported by ALPHA-M, are less than the calculated average error in photopeak positioning. For example, in a set of 400 spectra made by SIMSPEC with no shifts imposed, the average gain factor (1.000) and threshold shift (-0.23) are very close to ideal values determined earlier. This result indicates no inherent instability in the gain or threshold shift algorithm. Any apparent increase in analytical accuracy deriving from the application of automatic shifting may be due less to the actual shifting than to the use of this translational degree of freedom in accounting for the slight variations caused by counting statistics.

Since there is no evidence that it is detrimental to the final analytical results, use of the gain and threshold shift option may be worthwhile. The activity levels at which gain and threshold shifts can yield marked improvements in results have not been determined, but the routine use of shifting may have shifting invoked when these levels are indeed present in a sample.

Therefore, a summary of processing options can be recommended for routine use:

1. Compensate for background with a background library standard.

2. Use Y_c^{-1} as the weighting scheme.

3. Allow automatic compensation for gain and threshold shifts.

6.3 LIBRARY STANDARDS

After the program processing options are fixed, the performance of ALPHA-M will depend primarily on the library standards created for use with the least-squares process in spectra fitting. The primary consideration in creating a library of standards for use over a relatively long period of time is the stability of the spectrometer system. As far

TABLE 4. GAIN SHIFT EFFECTS
NUCLIDE ACTIVITIES 10 pCi/LITER

Nuclide	-1.5% Shift	No Shift	+1.5% Shift
	Weights based on $(Y_C)^{-1}$		
	%E[a]	%E	%E
^{131}I	89.0	70.0	68.1
^{134}Cs	54.9	66.0	68.7
^{137}Cs	60.4	57.2	57.3
^{54}Mn	68.7	53.0	64.6
^{60}Co	87.6	60.0	58.0
^{58}Co	146.0	83.7	69.2
^{140}Ba	77.0	85.7	82.9
^{106}Ru	153.0	105.0	128.0
^{95}Zr	140.0	138.0	133.0
	Weights based on $(DY_C)^{-1}$		
^{131}I	88.3	70.0	73.6
^{134}Cs	53.7	66.0	67.8
^{137}Cs	61.0	57.2	55.3
^{54}Mn	62.7	53.0	63.7
^{60}Co	54.2	60.0	55.6
^{58}Co	148.0	83.7	88.3
^{140}Ba	75.0	85.7	88.9
^{106}Ru	151.0	105.0	144.0
^{95}Zr	140.0	138.0	129.0

[a] $\%E = \%\ \text{Error} = \left|\frac{\text{Known-Found}}{\text{Known}}\right| \times 100$

as possible, all standards and sample spectra must be determined under an identical set of experimental conditions.

Factors such as system gain, linearity, and counting geometry must be maintained through rigorous quality control procedures. Changes in the counting system require restandardization followed by a reevaluation of the library.

The selection of members for the standard library for a particular analysis has a great deal to do with the performance of ALPHA-M. Therefore, after the library is created, the relationships among members must be determined. The first step in this process is to analyze a background spectrum using the full library. When the run is made, the correlation coefficients should be printed out as in table 5. These correlations reflect the interference or interaction of nuclides in the least-squares calculations. These coefficients are calculated from the inverted matrix from ALPHA-M and are equal to

$$\frac{A_{ij}^{-1}}{(A_{ii}^{-1})^{\frac{1}{2}}\,(A_{jj}^{-1})^{\frac{1}{2}}}\,, \tag{7}$$

where A_{ij} represents the matrix elements.

In least-squares analysis, the independent variables ideally should be mutually orthogonal; where this is not the case, the least-squares model will be weakened by interference in the process of refinement and greater inaccuracies will be included in the final results.

A survey of the correlation coefficients will indicate possible interfering pairs by showing values of greater than 0.6. High correlations may occur occasionally because of large fluctuations in counting statistics; but in general, the correlation matrix from a background sample will present a definite pattern. The analyses shown in table 6 were made during the course of this study using the standard library included in Appendix D. Examination of the correlation matrix will indicate possible sources of poor analytical performance among the selected standards.

These studies should be followed by analysis of gamma-ray spectra of composite samples containing combinations of the standard library radionuclides in known amounts. Satisfactory analytical results are a function of the criteria used by the analyst. One set of criteria for water samples has been set up by the Environmental Protection Agency in its gamma-in-water crosscheck program.[5] The one

TABLE 5. CORRELATION COEFFICIENTS FOR STANDARD NUCLIDE LIBRARY

	Background	^{144}Ce	^{51}Cr	^{131}I	^{106}Ru	^{134}Cs	^{137}Cs	^{95}Zr	^{58}Co	^{54}Mn	^{65}Zn	^{60}Co	^{40}K	^{140}Ba	Radon	Gain	Threshold
Background	1.000																
^{144}Ce	-0.191	1.000															
^{51}Cr	0.036	0.016	1.000														
^{131}I	0.055	-0.025	-0.001	1.000													
^{106}Ru	-0.291	-0.072	-0.041	0.013	1.000												
^{134}Cs	0.044	0.148	0.203	0.341	-0.102	1.000											
^{137}Cs	-0.314	0.026	-0.029	-0.004	-0.082	-0.049	1.000										
^{95}Zr	-0.291	-0.025	-0.063	-0.057	0.236	-0.276	0.049	1.000									
^{58}Co	0.052	-0.051	-0.087	-0.182	-0.265	-0.468	0.070	-0.283	1.000								
^{54}Mn	-0.150	0.018	0.027	0.050	0.334	0.096	-0.032	0.338	-0.794	1.000							
^{65}Zn	-0.127	0.083	0.057	0.134	-0.056	0.113	0.044	-0.012	-0.059	-0.007	1.000						
^{60}Co	-0.437	0.151	0.090	0.135	0.176	0.065	0.125	0.077	-0.077	0.084	-0.187	1.000					
^{40}K	-0.592	0.095	-0.004	0.032	0.203	-0.026	0.200	0.179	-0.032	0.085	0.035	0.141	1.000				
^{140}Ba	-0.631	0.131	-0.104	0.056	-0.081	0.128	0.229	0.120	-0.179	0.062	0.105	0.163	0.327	1.000			
Radon	-0.529	-0.092	-0.350	-0.557	0.051	-0.546	0.092	0.198	0.291	-0.049	-0.136	0.031	0.213	0.182	1.000		
Gain	0.126	-0.175	-0.031	0.207	0.065	0.057	-0.022	-0.024	-0.037	0.032	-0.015	0.017	-0.143	-0.116	-0.138	1.000	
Threshold	-0.172	0.246	0.109	-0.317	-0.067	-0.071	-0.040	0.008	0.032	-0.001	-0.002	0.011	0.114	0.116	0.192	-0.822	1.000

TABLE 6. OCCURRENCES OF HIGH CORRELATIONS IN A SET OF 132 ANALYSES[a]

Correlated Pair	No. of Occurrences	% of Total
^{54}Mn-^{58}Co	131	99.2
^{134}Cs-^{95}Zr-Nb	30	22.7
^{58}Co-^{106}Ru	9	6.8
^{58}Co-^{95}Zr-Nb	2	1.5
^{131}I-^{51}Cr	2	1.5
^{106}Ru-^{54}Mn	2	1.5
^{40}K-^{60}Co	2	1.5
^{134}Cs-^{106}Ru	1	0.8
^{134}Cs-^{58}Co	1	0.8
^{137}Cs-^{106}Ru	1	0.8
^{95}Zr-Nb^{106}Ru	1	0.8
^{65}Zn-^{60}Co	1	0.8

[a]Correlations between certain nuclides can be increased to importance on occasion, if large fluctuations in background or counting statistics occur.

standard deviation limit is 5 pCi/ℓ, if the activity is less than 100 pCi/ℓ, or 5 percent, if the activity is greater than 100 pCi/ℓ. It is true that these limits are established only for the case of a single nuclide; however, cases in which several nuclides are present are so complex that these values are used as a reasonable approximation. Analytical results for a composite are given in table 7; these results correspond very closely to the known values.

Selected single nuclide spectra can be analyzed for those nuclides having interference problems or those nuclides quantified inadequately in the composite samples such as the ^{106}Ru value for detector D in table 7. Poor performance with the individual nuclide spectra indicates possible problems with particular standard spectra. After all analytical problems are solved using known samples, the standards may be more fully evaluated for the type of analytical performance that may be expected in routine operation of the program.

The next step in testing the standard library is to examine the analytical results from the analysis of a large number of background spectra. Statistical fluctuations of the background counting rate should lead to a distribution of analytical results for each radionuclide in the standard library. Table 8 shows the distributions resulting from the analysis of 23 such background spectra. The library used with ALPHA-M to determine these values is not the one listed in Appendix D.

Ideally, all the radionuclides in the library should show a distribution with a mean value not significantly different from zero. A departure from zero could have several possible causes such as contamination of the shield, insufficient spectrometer stability, or uncompensated radon fluctuations in the counting room. All these factors could result in a larger background variability than that allowed from counting statistics only.

Overall, the agreement is good except for the isotopes ^{134}Cs, ^{58}Co, and ^{54}Mn. What nonideal properties of real data cause these discrepancies is an important question. An obvious contributor to the ^{58}Co-^{54}Mn anomalies is the correlation shown in table 6. Figure 8 better illustrates this correlation in action with the real analytical results. The anomalous ^{134}Cs, ^{58}Co, and ^{54}Mn results may also be related to the fact that these isotopes have, as shown later in this section, the lowest usable fractions in the library.

Radon and its daughter products present the most difficult problems in the ALPHA-M data analysis technique. Figures 9 and 10 illustrate the improvement that can be made in analytical results by including a simple radon standard

TABLE 7. ANALYTICAL RESULTS FROM COMPOSITE ANALYSIS

Nuclide	Known (pCi/ℓ)[a]	Found (pCi/ℓ)[b]			
		Det A	Det B	Det C	Det D
^{131}I	67±15	69±7	66±6	61±6	65±6
$^{103-106}Ru$	92±15	97±26	110±24	89±25	140±24
^{134}Cs	95±15	106±8	105±6	101±7	95±7
^{137}Cs	130±20	113±7	110±6	113±7	125±7
^{95}Zr-Nb	269±40	249±9	263±8	251±8	242±8
^{54}Mn	37±15	50±7	34±6	40±6	38±10
^{65}Zn	83±15	65±12	67±11	70±12	74±11
^{60}Co	102±15	97±15	95±5	96±5	91±5
^{140}Ba-La	76±15	69±6	72±5	66±5	73±5

[a]Amount added to the composite with the 3-sigma error as allowed by the criteria: <100 pCi/ℓ activity = 1σ = 5 pCi/ℓ
>100 pCi/ℓ activity = 1σ = 5%

[b]Result reported by ALPHA-M with the program standard error.

TABLE 8. EXPERIMENTAL VALUES DIVIDED BY STANDARD ERROR FOR 23 BACKGROUND SPECTRA

^{144}Ce	^{51}Cr	^{131}I	^{106}Ru	^{58}Co	^{134}Cs
-7*[a]	*	*	*	*	*
-6*	*	*	*	*	*
-5*	*	*	*	*	*1
-4*	*	*	*	*15	*9
-3*	*	*4	*6	*7	*6
-2*0	*00	*367	*	*1113	*2367
-1*0116	*3	*134	*12568	*239	*5
-0*13567	*1355789	*2579	*3679	*235	*366
0*112333455679	*26678	*03589	*012346	*57889	*59
1*6	*122	*69	*0123	*0111	*189
2*	*11346	*026	*02	*7	*
3*	*	*7	*8	*	*
4*	*	*	*	*	*
5*	*	*	*	*	*68
6*	*	*1	*	*	*
7*	*	*	*	*	*13

^{137}Cs	^{95}Zr-Nb	^{54}Mn	^{65}Zn	^{60}Co	^{40}K	^{140}Ba
-7*	*	*	*	*	*	*
-6*	*	*	*	*	*	*
-5*	*	*	*	*	*	*
-4*	*	*	*	*	*	*
-3*	*	*	*	*	*	*
-2*346	*42	*	*4	*68	*0015	*1
-1*023559	*017	*01278	*1335	*033	*6	*025
-0*12358	*045	*35	*57	*11246669	*013789	*0133679
0*1266	*012355677	*02223357	*124799	*12368	*2334579	*0112445689
1*05673	*012348	*134	*05557	*1358	*1258	*38
2*	*	*358	*01124	*0	*5	*
3*	*	*29	*	*	*	*
4*	*	*	*	*	*	*
5*	*	*	*	*	*	*
6*	*	*	*	*	*	*
7*	*	*	*	*	*	*

[a]The values are represented by two digits, the integer part and the first decimal. The digit to the left of the asterisk, shown only in the leftmost column, gives the integer part. Each digit on the right of the asterisk is the decimal part of one of the values. For example, entries for ^{58}Co on the -1 row are -1.2, -1.3, and -1.9.

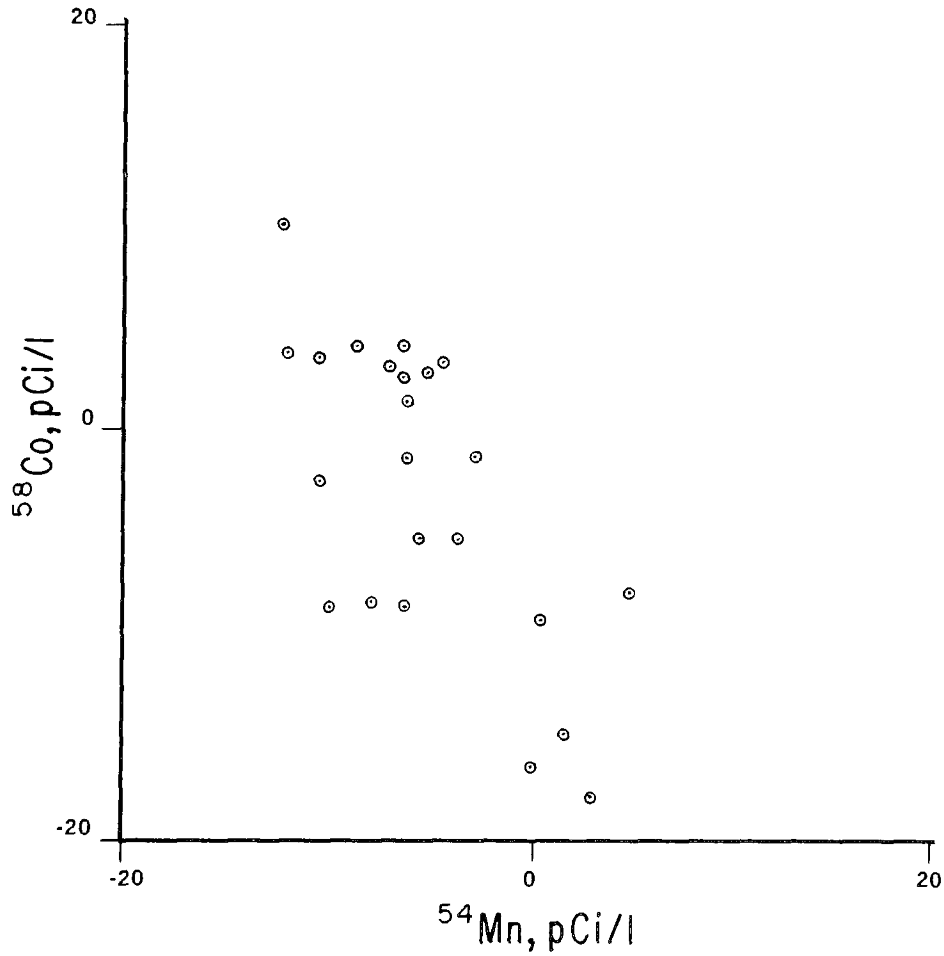
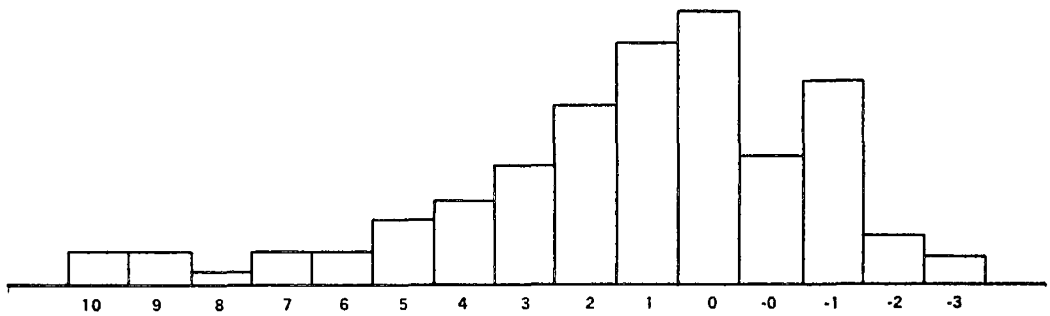


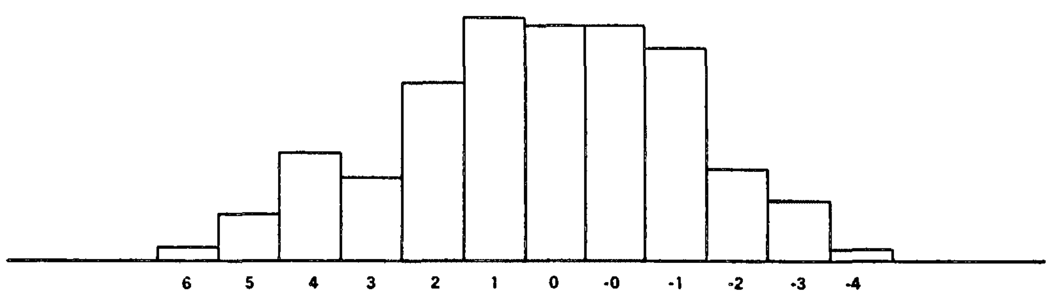
Figure 8. ^{58}Co activity vs. ^{54}Mn activity for background runs.

A. NO RADON STANDARD IN LIBRARY



(Decade)

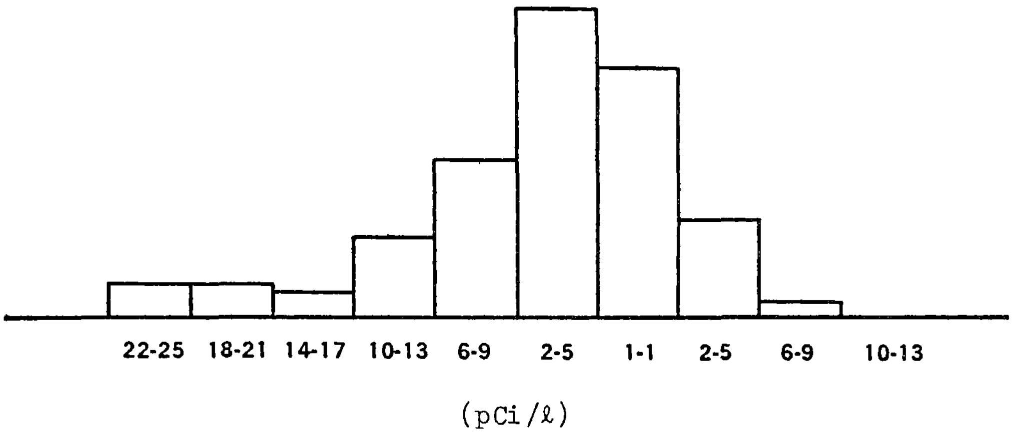
B. RADON STANDARD IN LIBRARY



(Decade)

Figure 9. ^{51}Cr sample results (pCi/ℓ).

A. NO RADON STANDARD IN LIBRARY



B. RADON STANDARD IN LIBRARY

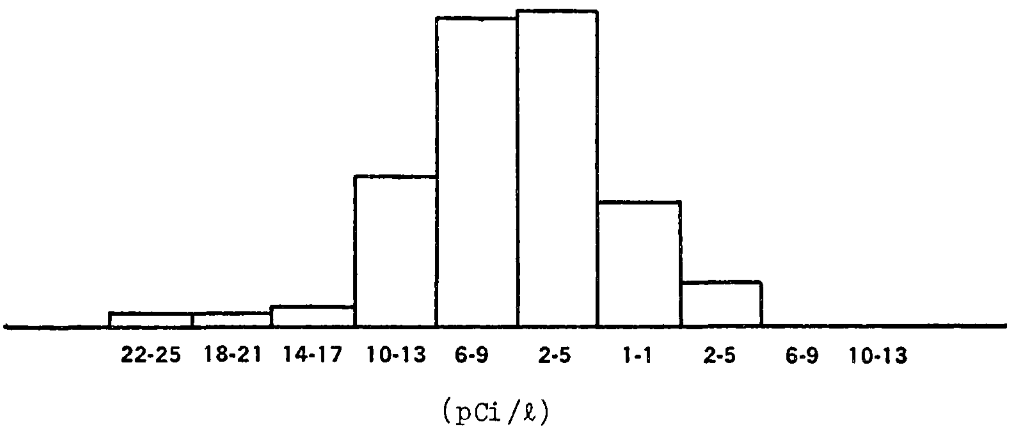


Figure 10. ^{134}Cs sample results (pCi/ℓ).

(radium in equilibrium with its short-lived decay products) in the library. In the set of library standards included in Appendix D, radon can interfere with the analysis of ^{51}Cr, ^{131}I, ^{134}Cs, and ^{65}Zn.

A single radon standard that has been allowed to reach equilibrium cannot completely account for all the radon daughter interferences that may be present in a sample. If the interference is not in equilibrium, then a standard in equilibrium will improve some radionuclide results and bias others. A possible solution for this problem is to make two library standards, one for ^{214}Pb and one for ^{214}Bi. These standards can then allow ALPHA-M to compensate for variations in the radon equilibrium.

After the standard library has been properly prepared and tested and is performing satisfactorily, the ultimate capability of the analysis system can be evaluated by using the standard errors calculated by ALPHA-M. These standard errors are obtained from the inverse of the ALPHA-M information matrix. The diagonal elements of the inverse matrix are the variances of each respective component, and the standard error of a component is simply the square root of its variance.[6]

For the Y_c^{-1} weighting option, the standard errors for any situation can be calculated after the nuclide and background levels have been specified. Let the count in channel i for standard j be given by X_{ij}. Let W_i be the weight chosen for channel i. Then the (i,j) element of the information matrix is given by

$$\sum_{i} X_{ii} W_i X_{ij} \quad . \qquad (8)$$

If a laboratory attempts to minimize background fluctuations, the only component necessary for consideration with environmental samples, where essentially no nuclide is presented, is the background library standard. Thus, an evaluation of ALPHA-M can be derived from the information matrix using weights given by the inverse of the background standard.

The library background spectrum is submitted to ALPHA-M for analysis. The full library, including the background standard itself, is used in analyzing the spectrum; no gain or threshold compensation is applied. Printouts of all matrix information should be requested. Tables 9 and 10 provide the resulting information matrix and inverse matrix respectively.

TABLE 9. **INFORMATION MATRIX**

(Multiply Values by 10^6)

^{144}Ce	2.40	0.19	0.35	0.57	0.41	1.24	0.90	0.68	0.72	0.45	1.08	0.56	7.86	0.134
^{51}Cr	0.19	0.16	0.11	0.15	0.12	0.36	0.22	0.20	0.22	0.13	0.32	0.14	2.73	0.039
^{131}I	0.35	0.11	0.46	0.34	0.27	0.87	0.56	0.48	0.48	0.29	0.70	0.29	4.82	0.083
^{106}Ru	0.57	0.15	0.34	1.04	0.62	1.76	1.15	0.81	0.96	0.66	1.43	0.57	10.53	0.150
^{58}Co	0.41	0.12	0.27	0.62	1.16	2.40	0.70	1.29	2.28	0.63	1.52	0.54	9.99	0.133
^{134}Cs	1.24	0.36	0.87	1.76	2.40	8.12	2.61	4.63	4.16	1.83	4.48	1.75	25.74	0.415
^{137}Cs	0.90	0.22	0.56	1.15	0.70	2.61	5.81	1.27	1.34	0.94	2.23	0.88	12.59	0.236
^{95}Zr-Nb	0.68	0.20	0.48	0.81	1.29	4.63	1.27	4.39	1.73	0.98	2.32	0.89	13.79	0.218
^{54}Mn	0.72	0.22	0.48	0.96	2.28	4.16	1.34	1.73	6.82	1.22	2.91	1.05	19.03	0.258
^{65}Zn	0.45	0.13	0.29	0.66	0.63	1.83	0.94	0.98	1.22	2.73	3.03	0.90	10.25	0.175
^{60}Co	1.08	0.32	0.70	1.43	1.52	4.48	2.23	2.32	2.91	3.03	11.96	2.44	27.33	0.458
^{40}K	0.56	0.14	0.29	0.57	0.54	1.75	0.88	0.89	1.05	0.90	2.44	2.25	10.27	0.187
^{140}Ba	7.86	2.73	4.82	10.53	9.99	25.74	12.59	13.79	19.03	10.25	27.33	10.27	217.65	0.247
Bkgd.	0.134	0.039	0.083	0.150	0.133	0.415	0.236	0.218	0.258	0.175	0.458	0.187	0.247	0.038

TABLE 10. INVERSE OF INFORMATION MATRIX

(Multiply Values by 10^{-6})

^{144}Ce	0.55	-0.15	0.02	-0.02	-0.14	0.08	0.01	-0.02	0.03	0.03	0.04	0.06	0.02	-4.26
^{51}Cr	-0.15	9.25	-0.48	0.36	-0.13	0.18	0.07	0.01	0.09	0.10	0.19	0.32	-0.02	-15.02
^{131}I	0.02	-0.48	4.20	-0.01	-0.34	0.19	0.04	-0.07	0.10	0.13	0.18	0.42	0.07	-19.21
^{106}Ru	-0.02	0.36	-0.01	2.88	-1.20	-0.08	-0.13	0.29	0.38	-0.05	0.15	0.26	-0.02	-11.21
^{58}Co	-0.14	-0.13	-0.34	-1.20	5.79	-0.92	0.07	-0.25	-1.30	-0.08	-0.15	-0.25	-0.10	15.38
^{134}Cs	0.08	0.18	0.19	-0.08	-0.92	0.80	0.00	-0.41	0.05	0.05	0.05	0.11	0.04	-7.97
^{137}Cs	0.01	0.07	0.04	-0.13	0.07	0.00	0.25	0.00	-0.01	0.02	0.02	0.06	0.02	-2.99
^{95}Zr-Nb	-0.02	0.01	-0.07	0.29	-0.25	-0.41	0.00	0.65	0.15	-0.02	0.01	0.02	-0.01	0.06
^{54}Mn	0.03	0.09	0.10	0.38	-1.30	0.05	-0.01	0.15	0.54	0.00	0.04	0.08	0.01	-3.78
^{65}Zn	0.03	0.10	0.13	-0.05	-0.08	0.05	0.02	-0.02	0.00	0.57	-0.07	0.02	0.01	-3.33
^{60}Co	0.04	0.19	0.18	0.15	-0.15	0.05	0.02	0.01	0.04	-0.07	0.20	0.04	0.01	-4.65
^{40}K	0.06	0.32	0.42	0.26	-0.25	0.11	0.06	0.02	0.08	0.02	0.04	0.90	0.04	-11.03
^{140}Ba	0.02	-0.02	0.07	-0.02	-0.10	0.04	0.02	-0.01	0.01	0.01	0.01	0.04	0.02	-2.13
Bkgd.	-4.26	-15.02	-19.21	-11.21	15.38	-7.97	-2.99	0.06	-3.78	03.33	04.65	-11.03	-2.13	479.93

The standard errors are the square roots of the diagonal elements of the inverse matrix multiplied by (1) the activities of the standard spectra and (2) a volume reduction factor of 1/3.5 (3.5 liters of water are normally counted). No correction is made for counting time since the sample and standards are counted for the same time period. No decay corrections are applied. Table 11 contains the resulting standard errors. (These are the standard errors used to compute table 8.)

The error estimates given by the ALPHA-M output (uncorrected for decay) differ in only two ways from the standard errors obtained above: (1) The information matrix used for the error estimates is the result of the ALPHA-M iteration; (2) the error estimate contains an additional factor equal to the square root of the CHDF. If the fit is good, CHDF approximates unity. Thus, except for high-activity samples, the measure of fit and standard errors such as those in table 11 provide the same information as the routine error estimates produced by ALPHA-M. To illustrate the close correspondence of the routine values to those obtained theoretically, table 12 contains the ALPHA-M error estimates for ten background spectra taken over a two-week period.

Closer examination of the standard error term shows that it can be expressed as the product of four factors: (1) the reciprocal of the specific area; (2) the reciprocal of the shape factor; (3) the reciprocal of the square root of the usable fraction; and (4) scale factors such as the volume adjustments, time adjustments, and decay factor. The specific area is the total counts (the sum over all channels) for the standard divided by the activity of the standard in pico-Curies. This factor measures the number of disintegrations that result in counts and thus reflects such things as sample geometry and detector efficiency. The shape factor is the square root of the diagonal element of the information matrix divided by the total counts and is proportional to the standard error that would apply if no other nuclides were being sought in the analysis and if the true background spectrum were subtracted from the sample before analysis. The shape factor measures the sharpness and number of the photopeaks and their relation to the background spectrum. For example, the shape factor accounts for the fact that a nuclide with all its counts in one channel would be easier to detect than a nuclide with the same number of counts but with a spectrum more like the background spectrum. The usable fraction measures the way that the nonorthogonality of the standard spectra affects the standard error.[7] If the standards were orthogonal, the usable fractions would be equal to one. Other things being equal, the lower the usable fraction, the higher the standard error. The usable fraction can be computed from the information matrix and its inverse. For the jth

TABLE 11. STANDARD ERRORS AND LOWER LIMITS OF DETECTION (LLD) FOR THE STANDARDS LIBRARY IN APPENDIX D

Nuclide	Standard Error	LLD
^{144}Ce	10.08	33.16
^{51}Cr	17.97	59.12
^{131}I	2.31	7.60
^{106}Ru	8.69	28.59
^{58}Co	3.95	13.00
^{134}Cs	2.45	8.06
^{137}Cs	2.31	7.60
^{95}Zr-Nb	2.90	9.54
^{54}Mn	3.00	9.87
^{65}Zn	3.53	11.61
^{60}Co	1.93	6.35
^{40}K	30.18	99.29
^{140}Ba-La	3.09	10.17

TABLE 12. ALPHA-M STANDARD ERRORS FOR 10 ANALYSES OF ROUTINE BACKGROUND SPECTRA

Nuclide	Standard Error									
	1	2	3	4	5	6	7	8	9	10
^{144}Ce	9.64	9.45	8.40	8.80	9.14	8.47	9.04	10.27	8.17	10.37
^{51}Cr	18.32	18.88	15.65	16.82	18.33	16.02	16.90	19.68	16.98	17.50
^{131}I	2.78	2.81	2.36	2.69	2.72	2.77	2.64	3.21	2.48	3.15
^{106}Ru	10.05	9.96	8.75	9.54	9.42	9.46	9.46	10.88	8.81	10.89
^{134}Cs	3.14	2.88	2.75	2.95	2.82	2.83	2.94	3.44	2.56	3.46
^{137}Cs	2.31	2.11	1.97	2.20	2.04	1.92	2.09	2.50	1.90	2.38
^{95}Zr-Nb	2.59	2.49	2.17	2.36	2.41	2.14	2.33	2.68	2.20	2.76
^{58}Co	5.06	4.12	4.29	4.48	3.98	4.40	4.65	5.12	3.65	4.63
^{54}Mn	3.84	2.94	3.27	3.41	2.78	3.39	3.54	3.82	2.58	3.15
^{65}Zn	4.56	4.56	3.99	4.17	4.18	4.04	4.44	4.69	3.86	5.12
^{60}Co	2.12	2.12	1.80	1.81	2.02	1.78	1.94	2.07	1.85	2.37
^{40}K	31.77	33.09	27.22	26.46	31.61	29.11	29.05	30.29	28.79	34.99
^{140}Ba-La	2.51	2.36	2.09	2.00	2.22	2.09	2.32	2.36	2.09	2.58

nuclide, the usable fraction is given by the reciprocal of the product of element (j, j) of the information matrix and the element (j, j) of the inverse of the information matrix. Table 13 gives values for the shape factors, usable fraction, and specific area of the standard library in Appendix D.

An analysis similar to that given in table 13 can impart direct information to the user on the results to be expected in routine analysis. Nuclides with low specific areas or low usable fractions will be much more difficult to detect at very low levels. In addition, low values for these parameters could possibly lead to erratic results at near-zero activity levels. The analyst can also improve his work by selectively choosing his library members. Unfortunately, what the analyst must analyze for is not always a matter of choice.

The standard errors in table 11 have two important uses: (1) to determine a threshold level high enough that a reported activity above this level has little chance of being the result of a zero-activity sample; (2) to determine a lower limit of detection (LLD) at a sufficiently high value of the true activity that detecting that quantity of the nuclide has a high probability.[8-10] A discussion of the difference between these two uses is worth a brief discussion. The determination of a threshold is concerned with whether a measurement has significant activity; for instance, to hold the chance of mistaking a zero-activity sample for one containing the nuclide to a 5 percent level, a threshold of 1.645 times the standard error is used. Determination of an LLD is concerned with whether a sample containing the nuclide will register enough counts to exceed the threshold. During the counting period, an abnormally low number of disintegrations may occur, thus resulting in a determination that does not exceed the threshold. To hold a 5 percent chance that the sample containing the nuclide will result in a measurement that exceeds the threshold, the sample must have a true activity of at least 3.290 times the standard error. Table 11 gives the LLD values derived for the standards in Appendix D; these values are calculated by ALPHA-M for each nuclide in each sample. Samples with true activities at the LLD value have a 95 percent probability of producing a measurement higher than the threshold set to hold the chance of the threshold being exceeded by a zero-activity sample to 5 percent. This criterion is used in this version of ALPHA-M.

This 95 percent confidence criterion is very rigorous. A more liberal criterion would be to allow a 25 percent chance of erroneously reporting activity when none is actually present and to keep the 5 percent requirement for missing activity when it is actually present. This criterion would

TABLE 13. SPECIFIC AREA, USABLE FRACTION, AND SHAPE FACTOR FOR THE LIBRARY STANDARDS IN APPENDIX D

Nuclide	Specific Area	Usable Fraction	Shape Factor
^{144}Ce	3.24	0.7527	0.0102
^{51}Cr	2.13	0.6837	0.0091
^{131}I	22.62	0.5228	0.0076
^{106}Ru	8.82	0.3327	0.0065
^{58}Co	24.39	0.1488	0.0077
^{134}Cs	44.37	0.1549	0.0067
^{137}Cs	15.21	0.6779	0.0099
^{54}Mn	18.53	0.2739	0.0098
^{95}Zr-Nb	17.89	0.3527	0.0093
^{65}Zn	11.15	0.6404	0.0091
^{60}Co	31.28	0.4283	0.0072
^{40}K	1.76	0.4938	0.0076
^{140}Ba-La	35.88	0.1985	0.0058

result in the LLD being 2.32 times as great as the standard error.

Actual results of ALPHA-M performance at environmental activity levels are presented in tables 14 and 15. The analyst must decide what degree of imprecision is satisfactory before setting limits on data reporting.

Further study was conducted to determine how the presence of more than one component in the sample spectrum could affect accuracy; the simulation program SIMSPEC was used for this work. Sample spectra, containing a standard background plus three, five, seven, or nine different nuclides, were generated. These four samples were each randomized six separate times and analyzed (vs. the complete library) by the Y^{-1} weighting scheme. Nuclide concentrations were 25 pCi/ℓ for each nuclide. The other processing options used are defined in Appendix D. The average absolute percent error (for each set of six replicates) for each nuclide was determined in each sample.

As more components are introduced into the sample spectrum, the relative accuracy decreases (table 16), thus agreeing with theoretical prediction.[9] However, the effect is minimal and the program is still performing adequately. Also shown in table 16 are the values for single nuclide spectra prepared and analyzed in the same manner as were the multicomponent spectra. All the spectra in this study were randomized to a level greater than predicted by three standard deviations in counting statistics to ensure representation of the worst case of counting statistics.

The minimal rise in percent error with increasing number of nuclides in the spectra does not imply that high concentrations of certain nuclides would not cause very large changes in these percent error values. These results are meaningful only when all nuclides are present at environmental levels.

ALPHA-M is a weighted least-squares routine modified to compensate for gain and threshold shifts and to allow the weights to depend on those isotopes that are actually present. A detailed description of ALPHA-M requires consideration of the consequences of these modifications. The efficient method of evaluation first determines (1) how ALPHA-M would behave if it were a weighted least-squares routine and (2) how the modifications make the behavior differ from that of weighted least squares. This two-step approach is efficient because the first step can be handled by theory whereas the second step requires only enough simulation to compare ALPHA-M with weighted least squares. The comparison should require relatively little simulation because the iterative process for finding the proper shifts

TABLE 14. ANALYTICAL RESULTS FOR ^{137}Cs AT LOW ACTIVITY LEVELS

Added (pCi/ℓ)		Found (pCi/ℓ) ± S.E.[a] No Rejection Applied (%Error)	Rejection Applied[b] (%Error)
2.81		1.85±1.95	---
		0.62±2.03	---
		1.62±1.71	---
		3.46±2.36	4.02±2.36
		1.70±1.82	---
	Average	1.85 (-34.2%)	--- (---)
5.61		4.30±1.86	4.97±1.74
		6.43±2.03	5.82±1.92
		2.14±1.94	2.33±1.89
		9.51±2.09	9.86±2.09
		5.14±2.04	5.97±1.96
		3.09±2.08	1.32±2.06
	Average	5.10 (-9.1%)	5.05 (-10.0%)
14.12		14.61±1.58	14.08±1.48
		17.54±2.41	17.20±2.20
		14.06±1.75	14.60±1.72
		14.60±2.24	15.05±2.05
		13.67±1.82	13.54±1.77
		14.34±2.07	15.23±1.95
	Average	14.80 (4.8%)	14.97 (6.0%)
21.20		19.07±2.27	19.46±2.20
		20.84±2.38	19.34±2.62
		24.26±2.54	25.22±2.39
		14.25±2.02	14.24±1.90
		15.41±2.27	17.48±2.27
		22.81±1.84	22.24±1.93
	Average	19.44 (-8.3%)	19.66 (-7.3%)
42.22		36.86±2.51	36.91±2.35
		38.20±2.47	39.15±2.36
		38.39±2.31	40.62±2.28
		38.98±2.61	39.59±2.54
		42.47±2.86	41.75±2.48
	Average	38.98 (-7.7%)	39.60 (-6.2%)

[a]S.E. = ALPHA-M standard error.

[b]^{137}Cs was rejected after the first ALPHA-M pass because the determined concentrations were less than the standard error.

TABLE 15. ANALYTICAL RESULTS FOR ^{65}Zn AT LOW ACTIVITY LEVELS

Added (pCi/ℓ)		Found (pCi/ℓ) ± S.E.[a] No Rejection Applied (%Error)	Rejection Applied[b] (%Error)
3.01		1.75±4.04	---
		10.09±5.13	9.22±4.60
		-1.55±4.81	---
		-2.38±3.80	---
		8.17±4.49	6.44±4.33
		11.65±3.82	10.31±3.71
	Average	4.62 (53.5%)	--- (---)
6.59		8.11±4.00	7.22±3.83
		4.43±4.33	3.36±4.31
		8.59±3.58	8.98±3.39
		5.75±4.02	4.05±3.80
		14.78±3.41	13.69±3.30
		9.62±4.54	9.00±4.46
	Average	8.55 (29.7%)	7.72 (17.2%)
16.55		25.23±4.95	23.07±4.65
		20.53±4.31	19.66±4.26
		15.76±3.71	14.93±3.45
		20.75±4.27	19.32±4.03
		14.64±3.47	15.16±3.34
		20.59±4.25	20.57±4.15
	Average	19.58 (18.3%)	18.79 (13.5%)
24.80		22.99±4.71	23.84±4.63
		25.21±4.81	25.14±4.56
		31.45±4.39	29.64±4.44
		22.25±4.12	22.34±3.93
		25.75±4.40	25.23±4.04
	Average	25.53 (2.9%)	25.24 (1.8%)
49.40		54.14±4.75	53.70±4.84
		51.91±5.35	51.89±5.13
		50.95±5.03	51.36±5.22
		40.46±4.86	41.57±4.78
		50.93±3.76	49.85±3.74
		46.24±4.90	46.04±4.74
	Average	49.11 (0.6%)	49.07 (0.7%)

[a]S.E. = ALPHA-M standard error.

[b]^{65}Zn was rejected after the first ALPHA-M pass because the determined concentrations were less than the standard error.

TABLE 16. EFFECTS UPON ACCURACY CAUSED BY MULTIPLE COMPONENTS

NUCLIDE ACTIVITY 25 pCi/ℓ

Sample	Nuclide (%Error[a])								
	^{131}I	^{134}Cs	^{137}Cs	^{54}Mn	^{60}Co	^{58}Co	^{140}Ba	^{106}Ru	^{95}Zr
(Obtained for Single Component Spectra)	26.2	26.4	23.7	20.6	24.3	42.7	35.5	50.4	54.3
1	26.7	27.7	24.5	--	--	--	--	--	--
2	28.3	29.1	24.6	21.8	25.1	--	--	--	--
3	32.4	29.1	24.9	28.3	24.5	54.4	39.1	--	--
4	35.7	29.1	25.7	28.8	24.8	58.1	40.0	59.8	61.6

[a]% Error = $\left| \frac{\text{Known-Found}}{\text{Known}} \right| \times 100$

and weights is designed to make ALPHA-M approximate weighted least squares.

6.4 SAMPLE ANALYSES

The main tool that the ALPHA-M user has for evaluating the analytical results produced by the program is the fit information provided in the program output. The CHDF value and the descriptive statistics for the residuals indicate the quality of the fit. ALPHA-M is designed for Poisson distribution of the counts in the sample, with means given by some linear combination of the library standards. The program is not designed to handle the variations in the sample that arise from variations in the radon level or from isotopes not included in the library. The residuals and the CHDF statistic may not handle such variations adequately. That the CHDF statistic sometimes indicates that the residuals are non-normal is not surprising, nor is it an indication that the analytical results are invalid.

To better estimate the analytical results on a continuing basis, the user should take several approaches. First, duplicate sample analysis on a daily basis can provide a good idea of the precision that the program is capable of obtaining. Frequent analysis of samples having known activity coupled with a crosscheck program involving other laboratories can serve as a check on the routine accuracy of the analytical results from ALPHA-M and the whole analysis system.

Samples yielding anomalous results should be recounted and resubmitted to ALPHA-M if abnormal background fluctuations are suspected. Careful scrutiny of results and the maintenance of distribution charts (table 8) for all nuclides will also assist in isolating unusual values. In addition, records should be kept for suspicious channels as identified by ALPHA-M. These data may point to the presence of previously unsuspected nuclides for which no library standard is available.

6.5 USE OF THE REJECTION PROCEDURE

ALPHA-M provides the option of specifying that a "rejection" process be used in its analysis. If this option is selected (via program input), the analysis is first performed in the normal manner with the specified number of refinement cycles. Then, those nuclides whose standard error is related to the absolute value of their determined activity in a specified manner are removed from consideration, and the analysis is repeated.

If a nuclide's standard error equals or exceeds the absolute value of its determined activity, it is removed from the reanalysis. This corresponds to the point at which the activity of the nuclide is not significantly different (at one standard deviation) from zero. The actual criterion by which a nuclide will be rejected from reanalysis may be adjusted via program input.

About 1350 analyses of SIMSPEC-generated spectra were performed using the rejection criterion. The results obtained before and after rejection were compared for accuracy to determine the effectiveness of the rejection scheme.

Because of the wide variation in accuracy over the entire body of analyses, the results were segmented into accuracy percentile decades, and the effect produced by rejection was determined for each decade. Table 17 shows the number of cases and the benefit derived from rejection for each percentile decade. For example, there were 126 analyses for which the error in the determination was between 50 and 60 percent; of this group, the standard rejection procedure improved the accuracy of the determination in 40 percent of the analyses.

Because the levels of activity commonly found in radiochemical analyses of environmental samples usually fall into the region in which greater than 70 percent error is common, the small percentage of cases in which the accuracy of the determination will be improved may reduce the advantages that can be produced by a rejection and reanalysis procedure using the standard criterion.

The expectation of an improvement in accuracy as a result of rejection and reanalysis is based primarily on the assumption that the reduced library size will introduce fewer errors due to unnecessary terms in the matrix of simultaneous equations. This conclusion is shown to be correct by the improvement noticed in samples exhibiting high accuracy and precision. In such cases, the rejection-reanalysis process serves as a further refinement cycle and is reminiscent of automatic stepwise-regression algorithms. Difficulties arise in applying this process to analyses with a relatively low accuracy. In these cases it is common for a nuclide to be rejected on the basis of an imprecise determination.

On first analysis, this possible rejection of valid data might be prevented by allowing the rejection of a nuclide only if its standard error is at a different level (i.e., equal to or greater than twice the magnitude of its determined activity). This criterion would decrease the occurrence of situations in which an existing nuclide is rejected because of poor precision, but would also result in

TABLE 17. BEHAVIOR OF THE REJECTION PROCESS

Accuracy Percentile Decade Range of % Error Observed	Number of Cases in Decade	Percentage of Cases Improved by Reanalysis after Standard Rejection
0-10	270	67
10-20	324	58
20-30	252	56
30-40	36	36
40-50	90	40
50-60	126	40
60-70	36	14
70-80	18	11
80-90	18	28
90-100	54	15
>100	126	23

a smaller decrease in library size. These two effects would tend to cancel each other.

However, there are also strong arguments for the use of a rejection procedure. One advantage of this procedure is illustrated by the case of ^{54}Mn-^{58}Co discussed earlier. These two nuclides are highly correlated and, as shown in figure 8, actual cases of a large activity for one nuclide and negative activity for the other occur. When the nuclide with negative activity is rejected and ALPHA-M makes a second pass, the result for the remaining nuclide is lowered substantially.

Another factor to consider is the inability to know what activity levels to expect in a sample. If a sample has an activity sufficient to achieve reasonable accuracy (<40 percent error), the rejection procedure will lead to improvement in the processing. Another approach is to use rejection, but to keep both the before- and after-rejection activities in a data base to be statistically studied at a later time.

6.6 REFERENCES

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APPENDIX A

ALPHA-M

A.1 GENERAL

This modified version of ALPHA-M has been prepared for execution on an IBM 370-165. An effort has been made to eliminate program features that depend on an IBM installation. The only installation feature in the program is a time-of-day clock used for writing the analytical results to the Fortran logical unit designated by IOPT. Users should consult the computer staff at their laboratory before using the example Job Control Language given in this appendix (table A-1).

At installations that have computing equipment other than IBM, changes may be necessary in the ALPHA-M program. Computing center staff should be consulted regarding program revision and information about which Systems Control Language to use. To increase the nuclide standards in each library to more than 20, to increase the number of detectors to more than 4, or to increase the number of data channels to more than 256 requires certain modifications to ALPHA-M. To modify ALPHA-M to use more than 20 library standards, subscripted variables dimensioned by NS must be changed to the proper size; the subscripted variables and their dimensions are given in Section A.3. Also, if standard libraries are created with GEN4, then appropriate changes must be made in GEN4; these changes are discussed in Appendix B.

To modify ALPHA-M to accept standard libraries having more than four detectors, subscripted variables dimensioned by NDETS must be changed appropriately. Again, GEN4 must be modified to create the proper libraries.

To modify ALPHA-M to analyze data with more than 256 channels, subscripted variables dimensioned by M must be changed. The use of the value 256 in program operations such as DO LOOP indices has been removed; instead, the indices are limited by the input value of M. Those parameters in GEN4 that are subscripted by M must also be modified.

A.2 ALPHA-M FILES

According to the input or processing options selected, ALPHA-M may require use of the following files.

TABLE A-1. JOB CONTROL LANGUAGE PROCEDURE RUNALPH

//RUNALPH	PROC
//ALPHA	EXEC PGM=ALPHAM,REGION=17ØK,TIME=2
//STEPLIB	DD DSN=ENV2Ø.RADLAB.SS622Ø3Ø.TLIB,DISP=SHR,UNIT=333Ø
//	VOL=SER=SYSUØ4
//FTØ2FØØ1	DD UNIT=SYSPL,DISP=(NEW,DELETE,DELETE),SPACE=(TRK,(1Ø,5))
//FTØ3FØØ1	DD DSN=ENV2Ø.RADLAB.SS622Ø3Ø.STDH20,DISP=SHR,UNIT=333Ø,
//	VOL=SER=SYSUØ4
//FTØ4FØØ1	DD DSN=&&RESID,UNIT=SYSPL,DISP-(NEW,PASS,DELETE),
//	SPACE=(TRK,(1Ø,1) RLSE),DCB=(RECFM=VBS,LRECL=78Ø,BLKSIZE=3124)
//FTØ5FØØ1	DD DDNAME=SYSIN
//FTØ6FØØ1	DD SYSOUT=A,DCB=(RECFM=FBA,LRECL=133,BLKSIZE=3Ø59),
//	SPACE=(CYL,(1,1),RLSE)
//FTØ9FØØ1	DD SYSOUT=A,DCB=*.FTØ6FØØ1,SPACE=(CYL,(1,1),RLSE)
//ANALYZE	EXEC PGM=ANALYZE,REGION=1ØØK
//STEPLIB	DD DSN=ENV2Ø.RADLAB.SS622Ø3Ø.TLIB,DISP=SHR,UNIT=333Ø,
//	VOL=SER=SYSUØ4
//FTØ2FØØ1	DD DSN=&&RESID,DISP=(OLD,DELETE,DELETE),UNIT=SYSPL
//FTØ6FØØ1	DD SYSOUT=A,DCB=(RECFM=FBA,LRECL=133,BLKSIZE=3Ø59),
//	SPACE=(CYL,(1,1),RLSE)
//RUNALPH	PEND

A.2.1 Standard Nuclide Library

This input file is always required. Refer to documentation regarding program GEN4 (Appendix B).

A.2.2 Auxiliary Output File

An output file is required if the ALPHA-M input variable IAUX is greater than zero. If this option is selected, a binary unformatted record is written on Fortran logical unit IAUX at the completion of each processing option. This record contains the ALPHA-M variables XIDT, R, YC, and YOBS. XIDT is the sample identification (eight bytes, alphanumeric), and R, YC, and YOBS are vectors (each dimensioned at 256) containing, respectively, the normalized residuals, the calculated spectrum derived by ALPHA-M, and the original sample spectrum. This information may be made available to other software for further analysis of the residuals, for plotting purposes, or for any other record keeping of processing functions. If this sequential file is stored on a 3330-type device with a

```
DCB=(RECFM=VBS,LRECL=780,BLKSIZE=3124),
```

each 3330 track may contain about 16 records.

A.2.3 Analytical Results File

An output file is required if the ALPHA-M input variable IOPT is greater than zero. If this option is selected, a binary unformatted record is written to Fortran logical unit IOPT at the end of each processing option. This record is written according to the following list:

```
TNAME, XIDT, IMAGE, ADATE, ANOUN, NT, (TISO(IT(J)),ZT(IT(J)),
                    STDT(IT(J)),J=1,NT).
```

TNAME is the sample header card; XIDT is the sample identification (eight bytes, alphanumeric); ADATE is the date of numerical analysis (eight bytes, alphanumeric in the form MM/DD/YY, month/day/year); ANOUN is the time of numerical analysis (eight bytes, alphanumeric in the form HH/MM/SS, hour/minute/second); TISO is a vector containing standard nuclide names; NT is the number of nuclides for which the analysis was performed; IT is a vector containing the library standard numbers for those NT nuclides; and ZT and STDT are vectors containing the determined activities and standard errors respectively. IMAGE is a five-digit number that reflects the processing options used for the sample analysis. Each digit denotes a different option. This is determined in the following manner: 10000*IABP + 1000*NB + 100*(NW+2) + 10*(KT+2) + 1*Q. For example, an IMAGE value of 21340 indicates that the sample was analyzed in the following fashion: (1) detector 2 standards were used, (2) background was subtracted, (3) the weighting scheme was the reciprocal of the calculated counts, (4) automatic gain and threshold shift was used, and (5) no rejection coefficient was applied.

The file created from these records is intended to be a temporary storage facility for information that will be transferred, after editing, to a permanent data base. As described above, each record will have a length of 28+NT*12 bytes, or a maximum length of 196 bytes. If this file is written to a 3330-type device with a

```
DCB=(RECFM=VBS,LRECL=200, BLKSIZE=3004)
```

providing 15 records of information per block, each 3330 track will contain a minimum of 60 records.

A.2.4 Alternate Printer File

An output file is required if the user requests print-plots of either the normalized residuals or the observed and calculated spectra. Subroutine RESIDU produces these plots with printer formatted write statements directed to Fortran logical unit 9. A DD card describing this unit as a SYSOUT=A data set should be included if either of these plots is requested.

A.3 GLOSSARY OF IMPORTANT ALPHA-M VARIABLES

A.3.1 Unsubscripted Variables

Variable	Definition
CH	$\sum \left(Y_{o_i} - Y_{c_i}\right)^2 / \left(\left\|Y_{c_i} + 0.1 + XMOD\right\| + BA_i{*}FX\right)$
CHDF	CH/DN
DN	Degrees of Freedom = MF - NZ - N + 1
DAY*	Decay time in days
F	Gain shift (multiplicative factor) per cycle of refinement
FM*	Format under which all sample and background spectra will be read
FP	Accumulated gain factor
FTT	Input value of gain factor
FS	Ratio of sample counting time/background counting time
FD	Decay factor, e^{-kt}
FX	FS^2
FTT*	Value of gain shift input manually
FAT	Ratio of standard counting time/sample counting time
IAUX*	Fortran logical unit for auxiliary data output
IABP*	Integer to control which detector set is used
IOPT*	Fortran logical unit for analytical data output

---

*These variables appear on the ALPHA-M control cards. Refer to Section 5.0 for additional information.

Variable	Definition
IRD*	Flag to control print-plotting of residuals and spectra
IPRINT*	Flag to control printing of matrix information
IS*	The numbers of the "N" library standards selected for analysis
KT*	Flag to control compensation technique to be used
M*	Number of channels in spectrum
MF*	Final channel to be used in computations
MS*	See page 5-7 for definition
MU*	Fortran logical unit for print-plots
N*	Number of nuclide standards from library to use in analysis. (This value is incremented and decremented during processing to serve as a pointer for the gain and threshold variables, if used.)
NIT*	Maximum number of cycles of least-squares refinement
NBA*	Flag to control printing of library standards
NZ*	First channel to be used for computations
NTS*	Fortran logical unit for standard library spectra
NTM*	Fortran logical unit for sample spectra and background
NH*	Flag to control printing of correlation coefficients
NDETS	Number of detector sets in library
NOPT*	Number of option cards (processing options)

*These variables appear on the ALPHA-M control cards. Refer to Section 5.0 for additional information.

Variable	Definition
CNBR*	Flag to control reading of background spectrum
NBS*	Flag to control background subtraction
NB*	Flag to control background subtraction for a given option
NW*	Flag to control weighting scheme application
NS	Number of library standards
Q*	Ratio upon which to base rejection, and flag to control whether to use previously calculated values of gain and threshold shift
QH*	Energy offset (in channels) between sample and standards
RE	$\left(Y_{o_i} - Y_{c_i}\right)$, the residual
RT	$\left(Y_{o_i} - Y_{c_i}\right)^2 / \left(\left\lvert Y_{c_i} + 0.1 + XMOD \right\rvert + BA_i * FX\right)$, standardized residual
SH	Accumulated energy zero channel per cycle of refinement
SHC	Energy threshold shift per cycle of refinement
SHCT*	Value of threshold shift input manually
SMSHC	Accumulated energy threshold shift
SI	The sum of the sample spectrum channel counts
SB	The sum of the background spectrum channel counts
TB*	The background counting time
TSA*	The sample counting time
T	$\left(Y_{o_i} - Y_{c_i}\right)^2$

*These variables appear on the ALPHA-M control cards. Refer to Section 5.0 for additional information.

Variable	Description
TMO	$\left\lvert Y_{c_i} + 0.1 + XMOD \right\rvert$
TMP	$\left\lvert Y_{c_i} + 0.1 + XMOD \right\rvert + BA_i{*}FX$
TE	$Y_{o_i} + BA_i{*}FX$
TT	$\left(Y_{o_i} - Y_{c_i}\right)^2 / \left(Y_{o_i} + BA_i{*}FX\right)$
VU	$\sum \left(Y_{o_i} - Y_{c_i}\right)^2$
VY	$\sum W_i \left(Y_{o_i} - Y_{c_i}\right)^2$; at end of each cycle, VY = VY/DN
VVV	$\sum \left(\left\lvert Y_{c_i} + 0.1 + XMOD \right\rvert + BA_i{*}FX\right)$
VM*	Volume multiplicative factor; calculated activity and standard error are multiplied by this factor to give results corrected for sample concentration before analysis
VRED*	Volume reduction factor; calculated activity and standard error are divided by this factor to give values corrected for analytical sample size
XLD	Lower limit of detection
XIDT*	Sample identification
XMOD*	Modifier for weighting scheme

*These variables appear on the ALPHA-M control cards. Refer to Section 5.0 for additional information.

A.3.2 Subscripted Variables

Variable (Dimensions)	Description
A(NS+2,NS+2)	Information matrix where $A_{k\ell} = \sum_{i=NZ}^{MF} S_{kij}*S_{\ell ij}\ W_i$ where j = constant value for a particular analysis
AC(NS,NDETS)	Matrix of standard nuclide activities
AT(NS+2)	Vector of alpha factors
B(NS+2)	Observation vector where $B_k = \sum_{i=NZ}^{MF} S_{kij}*Y_i*W_i$ where J = constant value for a particular analysis
BA(M)	Background spectrum vector
CC(NS+2)	Vector of correlation coefficients
DA(NS+2,NS+2)	Matrix in which A is stored prior to inversion so that identity matrix may be calculated
DER(M)	Vector of derivatives (dCounts/dChannel)
FM(20)	Format under which sample is to be read
HA(NS)	Vector of standard nuclide half-lives
IS(NS+2) IT(NS+2)	The numbers of, or positional flags for variables selected, depending on location in program
R(M)	Normalized residuals, $R_i + \left(Y_{o_i} - Y_{c_i}\right) / \left(Y_{c_i} + BA_i\right)^{\frac{1}{2}}$
S(NS,M,NDETS)	Matrix containing all standard nuclide spectra
SS(NS,NDETS)	Squares of the sum of channels NZ to MF for all standard nuclides
STD(NS+2)	Contains standard errors for calculated parameters
STDT(NS+2)	Report vector for standard errors

Variable (Dimensions)	Description
TST(NS)	Vector of counting times for standard nuclides
TISO(NS+2)	Vector of names for standard nuclides, ordered as in calculations
TISOT(NS+2)	Vector of standard nuclide names
TNAME(20)	Contains identification header
W(M)	Channel weights
XI(NS+2,NS+2)	Calculated identity matrix AA^{-1}, or DA A^{-1}
XPE(NS)	Work vector for coefficients of variance
XPET(NS)	Report vector for coefficients of variance
Y(M+1)	Input vector for sample spectrum
YC(M)	Y_c, vector for calculated sample spectrum
YT(M)	Holding vector for corrected sample spectrum
YOBS(M)	Y_o, holding vector for corrected sample spectrum
Z(NS+2)	Vector of calculated coefficients, $Z_k = \sum_{i=NZ}^{MF} A^{-1}_{k,i} * B_k$
ZT(NS+2)	Report vector for final activities
ZUC(NS+2)	Working vector for uncorrected activities
ZTUC(NS+2)	Report vector for uncorrected activities

A.4 IMPORTANT FORMULAE

$$\text{CHDF} = \frac{\sum \frac{\left(Y_{o_i} - Y_{c_i}\right)^2}{\left(Y_{c_i} + BA_i + 0.1\right)}}{DN}$$

$$\text{Activity of Nuclide}_i = Z_i * FAT * AC_i * FD * VM/VRED$$

$$\text{Std. Error of Nuclide}_i = \left[A^{-1}_{ii} * \frac{\Sigma WdY^2}{DN}\right]^{\frac{1}{2}} * FAT * AC_i * FD * VM/VRED$$

$$\text{Alpha-factor of Nuclide}_i = \left[A^{-1}_{ii} * \frac{\Sigma Wdy}{DN}\right]^{\frac{1}{2}} * \left[\frac{SS_i}{\Sigma dY^2}\right]^{\frac{1}{2}}$$

$$\text{C.V. of Nuclide} = 100 \text{ X } \underline{\text{Std. Error Nuclide}_i} / (\text{Activity Nuclide}_i)$$

$$\text{Correlation Coefficient of Nuclide with Nuclide} = \frac{\left(A_{ij}\right)^{-1}}{\left(A^{-1}_{ii}\right)^{\frac{1}{2}} * \left(A^{-1}_{jj}\right)^{\frac{1}{2}}}$$

A.5 ALPHA-M PROGRAM

The following is a computer printout of the program ALPHA-M.

ALPHA-M PROGRAM

```
C*****************************************************************************
C
C
C     ALPHA-M   MULTI-COMPONENT GAMMA-RAY SPECTRUM ANALYSIS
C     BASED ON THE PROGRAM WRITTEN BY EARNEST SCHOENFIELD, ORNL, 1965
C     CURRENT VERSION 2, LEVEL 3, MAY 1976, TENNESSEE VALLEY AUTHORITY
C     DIVISION OF ENVIRONMENTAL PLANNING, RADIOLOGICAL HYGIENE BRANCH
C     RIVER OAKS BUILDING, MUSCLE SHOALS, ALABAMA    35660
C
C
C*****************************************************************************
C
      REAL * 8 TISOT,TISO,XIDT,ADATE,ANOUN,D
      INTEGER * 4 FM,TNAME
      DIMENSION YZ(256),A(22,22),Y(257),Z(22),CC(22),STD(22),B(22),
     $           R(256),W(256),DER(256),YT(256),IR(256),BA(256),FM(8),
     $           SS(20,4),AC(20,4),HA(20),IS(22),TST(22),HAT(22),AT(22),
     $           STDT(22),TNAME(20),TISOT(22),TISO(22),IT(22),ZT(22),
     $           S(20,256,4),XPE(20),XPET(20),YC(256),XI(22,22),
     $           DA(22,22),ZUC(22),ZTUC(22),YOBS(256),STDUC(22).
     $           STTUC(22),XLD(20),XLDT(20)
      COMMON/STUFF/XIDT,TISOT,NS,M,NIT,NBA,NZ,MF,NH,KK,NTS,NTM,NQ,Q,FX,
     $           MS,NSAMP,NOPT,IPRINT,NBR,NBS,IABP,TB,ISA,VRED,DAY,VM,
     $           NBN,NB,NW,N,KT,LW,YOBS,K23D,QH,NDET,IS,MO,NRED,IN,FS,
     $          NBRI,FM,S,SS,AC,NDETS,HA,TST,Y,YC,IOPT,IAUX,R,XMOD,IRD,MU
C
C     IBM EXTENDED ERROR MESSAGE HANDLING FACILITY
C     TERMINATE JOB UPON SINGLE OCCURRENCE OF DEC-CHAR CONVERSION
C

C
      NRED=0
      NBR1 = 0
      MI=5
      MO=6
      DO 1 I =1,256
      YC(I)  0.0
      R(I) = 0.0
    1 BA(I)  0.0
C
      CALL DATE (ADATE,ANOUN)
C     SUBROUTINE DATE IS T.V.A. INSTALLATION DEPENDENT
      WRITE(MO,9901)ADATE,ANOUN
C
C     READ CONTROL CARD AND DATA FORMAT
C
    2 READ(MI,52) M,NIT,NBA,NZ,MF,NTS,NTM,MU,NH,IAUX,IOPT,FM
      CALL LABEL
      CALL DIAG
C
C     READ STANDARDS INFORMATION
C
      CALL STDIN
C
C     READ SAMPLE INFORMATION CARD
C
   17 READ(MI,65,END=180) XIDT,NOPT,NBR,NBS,IABP,MS,TB,TSA,VRED,DAY,VM
      IF (NBR.EQ.1) NBR1 = 1
C
C     DEFINE CONSTANTS VM,VRED,FS,FX
```

```
C
   18  IF (VM) 19,19,20
   19  VM=1.0
   20  IF (VRED) 21,21,22
   21  VRED=1.0
   22  IF (TB) 23,23,24
   23  FS=0.0
       GO TO 25
   24  FS=TSA/TB
   25  FX    FS**2
C
      CALL LABEL1
      CALL DIAG1
C
       IF(NBR) 27,27,26
C
C     READ BACKGROUND IDENTIFICATION
C
   26 PEAD(NTM,67)TNAME
      WRITE(MO,68) TNAME
C
C     READ BACKGROUND SPECTRUM
C
      READ(NTM,FM) BA
      WRITE(MO,61) BA
      WRITE(MO,64)
C
C     SWAP BKGND FOR LIBRARY STANDARD IF REQUESTED
C
      IF (MS.EQ.0) GO TO 27
      DO 261 I=1,M
261   S(MS,I,IABP) = BA(I)
      DO 263 J=1,NS
      SS(J,IABP)   0.0
      DO 262 I=NZ,MF
262   SS(J,IABP)   SS(J,IABP) + S(J,I,IABP)
263   SS(J,IABP) = SS(J,IABP) * SS(J,IABP)
C
C     READ SAMPLE IDENTIFICATION
C
      WRITE(MO,64)
   27 READ(NTM,67) TNAME
      WRITE(MO,68) TNAME
      NRED=NRED+1
C
C     READ SAMPLE SPECTRUM
C
      READ(NTM,FM) (Y(I),I=1,M)
C
C     CORRECT FOR NEGATIVE COUNTS
C
      DO 28 I=1,M
   28 IF (Y(I).GT.900000.0) Y(I) = Y(I) - 1000000.0
31    IF (NBS) 37,37,35
C
C     SUBTRACT BACKGROUND PERMANENTLY IF REQUIRED
C
   35  DO 36 I=1,M
   36  Y(I)=Y(I)-BA(I)*FS
C
```

```
C     CALCULATE BACKGROUND SUM
C
   37 SB=0.0
      DO 38 I=NZ,MF
   38 SB=SB+BA(I)
C
C     PRINT CORRECTED SAMPLE SPECTRUM
C
      WRITE(MO,61) (Y(I),I=1,M)
      S1=0.0
      S2=0.0
C
C     CALCULATE SAMPLE SUM
C
      DO 39 I=NZ,MF
   39 S1=S1+Y(I)
        S2=S1+SB*FX
C
C     PRINT BACKGROUND AND SAMPLE SUMS
C
      WRITE(MO,69) SB,S1
      DO 40 I=1,M
   40 YT(I)=Y(I)
C
C     START OPTIONS LOOP ------------------------------------------
C
      DO 169 IN=1,NOPT
C
C     READ OPTIONS CARD
C
      READ(MI,70) N,NB,NW,KT,IRD,IPRINT,QH,Q,XMOD,(IS(I),I=1,N)
      SH=-QH
      KK=0
      NTT=N
C
C     SETUP ORDERING ARRAYS FOR CALCULATIONS AND OUTPUT
C
      DO 43 J=1,N
      DO 42 I=1,NS
        IF(IS(J)-I) 41,41,42
   41     TISO(J)=TISOT(I)
        GO TO 43
   42   CONTINUE
   43 CONTINUE
      DO 44 J=1,NTT
   44 IT(J)=J
C
45    CALL LABEL2
      IF (KK.EQ.0) CALL DIAG2
C
      DO 46 J=1,M
   46 Y(J)=YT(J)
      IF(NB) 49,49,47
C
C     SUBTRACT BACKGROUND IF REQUESTED THIS OPTION
C
   47 DO 48 J=1,M
   48 Y(J)=Y(J)-BA(J)*FS
C
   49 DO 50 J=1,M
```

```
   50 YOBS(J) = Y(J)
      FP = 1.0
       SMSHC=0.0
      KT1 - KT + 1
      IF (KT1) 93,91,94
   91  IF (KK) 92,92,93
C
C     FOR MANUAL COMPENSATION, ENTER GAIN AND THR SHIFT VALUES
C
   92 READ(MI,56) FTT,SHCT
      WRITE(MO,56) FTT,SHCT
   93  CALL SHIFT (Y,M,SH,FTT,SHCT)
       FP=FTT
       SMSHC=SHCT
C
C     CALCULATE POINTERS FOR GAIN AND THR SHIFTS
C
  94  IS(N+1)    NS + 1
      IS (N+2) = NS + 2
       NT=N
       CHT= 1.0E20
C
C     START ITERATIONS LOOP ------------------------------------------
C
      DO 141 LO=1,NIT
       N=NT
       IF(NW) 96,96,95
C
C     IF WTS BASED ON CALC'D CTS, CALC INITIAL WTS FOR 1ST ITER ONLY
C
   95  IF(LO-1) 96,96,104
C
C     IF WTS BASED ON OBS'D CTS, CALC WTS HERE EVERY ITER.
C
   96  DO 101 I=1,M
      IF (IABS(NW)-2) 102,98,97
C
C     FOR UNIT WEIGHTING SCHEME
C
   97    W(I)=1.0
       GO TO 101
C
C     FOR 1/VAR WEIGHTING SCHEME
C
   98  T=Y(I)+BA(I)*FX
       IF (T- 1.0) 99,99,100
   99  W(I)=1.0
       GO TO 101
  100  W(I)=1.0/T
  101  CONTINUE
       GO TO 104
C
C     FOR 1/COUNTS WEIGHTING SCHEME
C
  102  DO 103 I=1,M
  103 W(I)    1.0/(ABS(Y(I)) + 1.5)
C
C
  104  IF (KT) 112,112,105
  105  N=N+1
```

```
      I=M-1
      N5=IS(N)
C
C     SETUP GAIN SHIFT VARIABLE
C
      DO 109 J=2,I
       C=J
      IF(Y(J+1)-1.0 ) 108,108,106
  106 IF(Y(J-1)-1.0 ) 108,108,107
  107 DER(J)=(Y(J+1)-Y(J-1))/2.0
      GO TO 109
  108 DER(J)=0.0
  109 S(N5,J,IABP)   -DER(J) * (C+SH)/100.0
         N5=IS(N)
      S(N5,1,IABP) - S(N5,2,IABP)
      S(N5,M,IABP) = S(N5,M-1,IABP)
      IF (KT-1) 112,112,110
  110 N=N+1
      I=M-1
      N5=IS(N)
C
C     SETUP THRESHOLD SHIFT VARIABLE
C
      DO 111 J=2,I
  111 S(N5,J,IABP) = -DER(J)
         N5=IS(N)
      S(N5,1,IABP) = S(N5,2,IABP)
      S(N5,M,IABP) = S(N5,M-1,IABP)
C
C     CREATE MATRIX A
C
  112 DO 115 L=1,N
        N5=IS(L)
         DO 114 K=L,N
          N6=IS(K)
          SA=0.
           DO  113 I=NZ,MF
  113 SA = SA + S(N6,I,IABP) * S(N5,I,IABP) * W(I)
                A(K,L)=SA
                A(L,K)=A(K,L)
  114    CONTINUE
  115 CONTINUE
C
C     CREATE VECTOR B
C
      DO 117 K=1,N
          N6=IS(K)
         SX=0.
        DO 116 I=NZ,MF
      SX - SX + S(N6,I,IABP) * Y(I) * W(I)
  116   CONTINUE
  117 B(K)=SX
      IF (IPRINT.EQ.0) GO TO 1500
C
C     PRINT INFORMATION MATRIX IF REQUESTED
C
      WRITE(MO,83)
      DO 1000 I=1,N
 1000 WRITE(MO,63) (A(I,J),J=1,N)
      DO 1001 I=1,N
```

```
      DO 1001 J=1,N
 1001 DA(I,J) = A(I,J)
C
C     INVERT MATRIX A
C
 1500 CALL INVERT (A,N,D)
C
      IF (IPRINT.EQ.0) GO TO 2000
C
C     PRINT INVERSE AND IDENTITY MATRIX IF REQUESTED
C
      WRITE(MO,82)
      DO 1003 I=1,N
 1003 WRITE(MO,63) (A(I,J),J=1,N)
      DO 1004 I=1,N
      DO 1004 J=1,N
 1004 XI(I,J)   0.0
C
C     CALCULATE IDENTITY MATRIX
C
      DO 1005 I=1,N
      DO 1005 J=1,N
      DO 1005 K=1,N
1005  XI(I,J) - XI(I,J) + A(I,K)*DA(K,J)
      WRITE(MO,86)
      DO 1006 I=1,N
 1006 WRITE(MO,63) (XI(I,J),J=1,N)
C
C     CALCULATE VECTOR Z   INV A * B
C
 2000 DO 119 J=1,N
          SUM=0.
          DO 118 I=1,N
          SUM=SUM+A(J,I)*B(I)
  118     CONTINUE
  119 Z(J)=SUM
      CH=0.0
      VY=0.
       CHS=0.0
       VU=0.0
       VVV=0.0
C
C     BEGIN LOOP TO CALCULATE ERROR SUMS, RESIDUALS, AND NEW WEIGHTS
C
      DO 128 J=NZ,MF
      SV   0.
      DO 120 I=1,N
      N5   IS(I)
  120 SV   SV + S(N5,J,IABP) * Z(I)
C
C     YC IS CALCULATED SPECTRUM
C
      YC(J)   SV
C
C     CALCULATE RESIDUAL   RE
C
       RE=Y(J)-SV
       T=RE**2
       VY=VY+W(J)*T
       VU=VU+T
```

```
      TMD - ABS(SV + 0.1 + XMOD)
      IF(TMD)183,184,183
  184 TMD = 1.0
  183 CONTINUE
C
C     CALCULATE VARIANCE OF CALCULATED COUNTS/CHANNEL
C
       TMP=TMD+BA(J)*FX
      IF(TMP)185,186,185
  186 TMP - 1.0
  185 CONTINUE
       VVV=VVV+TMP
       IF (NW) 124,124,121
C
C     IF WEIGHTING SCHEME BASED ON CALC'D COUNTS, ASSIGN NEW WEIGHTS HER
C
  121 IF (NW-2) 123,122,124
C
C     FOR WEIGHTS BASED ON RECIPROCAL VARIANCE (YCALC)
C
  122  W(J)=1.0/TMP
       GO TO 124
C
C     FOR WEIGHTS BASED ON RECIPROCAL YCALC
C
  123  W(J)=1.0/TMD
C
  124    RT=T/TMP
         CH=CH+RT
      TMP=SQRT(TMP)
C
C     CALCULATE VECTOR OF NORMALIZED RESIDUALS
C
         R(J)=RE/TMP
  128 CONTINUE
C
C     END LOOP FOR ERRORS, RESIDUALS, AND WEIGHTS
C
C     CALCULATE DEGREES OF FREEDOM AND FIT FACTORS
C
      DN = MF-N-NZ+1
      CHDF = CH/DN
      VY = VY/DN
C
C     CALCULATE STD DEV OF PARAMETERS
C
      DO 129 I=1,N
         E=A(I,I)*VY
      STD(I)= E
  129 CONTINUE
C
      IF (KT-1) 130,133,132
  130 WRITE(MO,73) CHDF
      IF (NW) 142,142,135
C
C     CALCULATE THRESHOLD AND GAIN SHIFT CONTRIBUTIONS
C
  132  NU=N-1
         SH=SH-Z(N)
          SHC= -1.0*Z(N)
```

```
      GO TO 134
  133  NU=N
        SHC= 0.0
  134  F=1.0-Z(NU)/100.0
       FP=FP*F
       SMSHC=SMSHC+SHC
      WRITE(MO,73) CHDF,SMSHC,FP
C
C     CHECK REFINEMENT PROCESS
C
  135  IF (NW) 136,136,139
C     IF WEIGHTS BASED ON OBS'D SPECTRUM ...
  136  T= (CHT-CH)/CH
C     ...STOP IF DIVERGING BY MORE THAN 5%
       IF (T+0.05) 142,142,137
C     ... STOP IF CONVERGING BY LESS THAN 5%
  137  IF (T- 0.05) 142,142,138
C     ... STOP IF CHDF LESS THAN 1.2
  138  IF ( CHDF - 1.2) 142,142,139
  139      CHT=CH
       IF(KT) 192,192,140
  140  CALL SHIFT (Y,M,SH,F,SHC)
C     FOR ALL WEIGHTING SCHEMES - STOP IF CHDF LESS THAN 0.3
  192 IF(CHDF -0.3)142,141,141
  141 CONTINUE
C
C     END ITERATIONS LOOP -------------------------------------------------
C
C     CALCULATE AND OUTPUT CORRELATION COEFFICIENTS
C
  142 IF (NH.EQ.0) GO TO 145
 9188 WRITE(MO,9903)
      DO 9190 I = 1,N
      DO 9189 J = 1,N
 9189 CC(J) - A(I,J)/(SQRT(ABS(A(J,J)))*SQRT(ABS(A(I,I))))
 9190 WRITE(MO,9902)I,(CC(K),K=1,I)
C
C     CALCULATE ALPHA FACTORS
C
  145  DO 143 I=1,NT
         N5=IS(I)
         N6=IT(I)
      IF(VU) 190, 191, 190
  191 A(I,I) = 0.0
      AT(N6) = 0.0
      GO TO 143
  190 CONTINUE
      A(I,I)   SS(N5,IABP) * A(I,I) * VY/VU
      AT(N6)   SQRT(ABS(A(I,I)))
  143 CONTINUE
C
C     CALCULATE FINAL STD ERRORS AND ACTIVITIES
C
       DO 144 I=1,NT
       N5=IS(I)
       HAT(I)=HA(N5)
      FD=EXP(0.693*DAY/HA(N5))
       FAT=TST(N5)/TSA
      STDUC(I) = FAT * AC(N5,IABP) * SQRT(STD(I)) * VM/VRED
      STD(I) - FAT * AC(N5,IABP) * FD * SQRT(STD(I)) * VM/VRED
```

```
      XLD(I) = STD(I) * 3.29
      ZUC(I) = Z(I) * FAT * AC(N5,IABP) * VM/VRED
      Z(I)   Z(I) * FAT * AC(N5,IABP) * FD * VM/VRED
      XPE(I) = ABS(((Z(I)-(Z(I)-STD(I)))/Z(I))*100.)
  144 CONTINUE
C
  146  DO 147 J=1,NT
      N5 = IT(J)
      ZT(N5)   Z(J)
      ZTUC(N5)   ZUC(J)
      STTUC(N5) = STDUC(J)
      XPET(N5) - XPE(J)
      XLDT(N5) = XLD(J)
  147 STDT(N5) = STD(J)
C
C     OUTPUT RESULTS
C
      WRITE               (MO,75)
      DO 1147 J=1,NT
      N5 = IT(J)
 1147 WRITE(MO,76) N5,TISO(N5),ZTUC(N5),STTUC(N5),ZT(N5),STDT(N5),
     $              XPET(N5),AT(N5),XLDT(N5)
C
       CALL RESIDU
C
      IMAGE   10000*(IABP) + 1000*(NB) + 100*(NW+2) + 10*(KT+2) + KK
C
C     WRITE AUX. OUTPUT AS REQUESTED
C
      IF (IAUX.GT.0) WRITE(IAUX) XIDT,IMAGE,R,YC,YOBS
C
C     WRITE DATA BASE OUTPUT AS REQUESTED
C
      IF (IOPT.EQ.0) GO TO 1148
      CALL DATE (ADATE,ANOUN)
      WRITE(MO,9904) ADATE,ANOUN
      WRITE(IOPT) TNAME,XIDT,IMAGE,ADATE,ANOUN,NT,
     $             (TISO(IT(J)),ZT(IT(J)),STDT(IT(J)),J=1,NT)
C
C     RE-ORDER ARRAYS IF REJECTION PROCEDURE UTILIZED
C
 1148 IF (Q) 156,169,148
  148  KK=KK+1
      IF (KK-2) 149,169,169
  149 DO 151 I=1,NT
      IF (Z(I)/STD(I) - ABS(Q)) 150,150,151
  150    IS(I)=0
  151  CONTINUE
       KR=0
      DO 153 J = 1,NT
         IF (IS(J)) 153,153,152
  152    KR=KR+1
       IS(KR)=IS(J)
       IT(KR)=J
  153  CONTINUE
       IF (KR) 154,169,154
  154  IF(KR-NT) 155,169,155
  155  N=KR
      SH = -QH
       GO TO 45
```

```
C
C     HEAD BACK TO RECALCULATE WITH REJECTION
C
  156  FTT=FP
       SHCT=SMSHC
C
  169 CONTINUE
C
C     END OPTIONS LOOP -----------------------------------------------------
C
  174 GO TO 17
  180 WRITE(6,176)
      STOP
C
C**********************************************************************
C
   52 FORMAT(11I4,8A4)
   56 FORMAT(2F10.4)
   61 FORMAT(1X,10F12.1)
   63 FORMAT(E14.6,E14.6,E14.6,E14.6,E14.6,E14.6,E14.6,E14.6,E14.6)
   64 FORMAT(1H1)
   65 FORMAT(A8,5I3,5F9.4)
   67 FORMAT(20A4)
   68 FORMAT (1X,18A4,2A8)
   69 FORMAT(12H BACKGD SUM=  F10.0,16H     SAMPLE SUM=  F10.0)
   70 FORMAT(6I3,3F6.2,(22I2))
   73 FORMAT(' CHDF    ',F6.2,'   THR SHIFT = ',F7.4,
     $'    GAIN SHIFT    ',F7.4)
   75 FORMAT(/,T3,'LIBRARY',T13,'NUCLIDE',T28,'DECAY UNCORRECTED',
     $ T55,'DECAY CORRECTED',T77,'COEFFICIENT',T93,'ALPHA',/,
     $ T3,'NUMBER',T13,'NAME',T26,'ACTIVITY     STD. ERR.',
     $ T52,'ACTIVITY     STD. ERR.',T77,'OF VARIANCE',T93,'FACTOR',
     $7X,'LLD')
   76 FORMAT(I6,6X,A8,4(4X,F9.4),6X,F6.2,7X,F7.4,5X,F8.4)
   82 FORMAT(/,' INVERSE MATRIX',/)
   83 FORMAT(/,' INFORMATION MATRIX',/)
   86 FORMAT(/,' IDENTITY MATRIX',/)
  176 FORMAT('0* * * * * * * ALPHA-M NORMAL TERMINATION * * * * * * * *')
 9901 FORMAT('OALPHA-M   VERSION 2   LEVEL 3          RADIOANALYTICAL',
     $' LABORATORY',12X,'DATE: ',A8,5X,'  TIME:',A8,///)
 9902 FORMAT(I4,16F8.3)
 9903 FORMAT(/,' CORRELATIONS ',/)
 9904 FORMAT(/,' SAMPLE/OPTION WRITTEN TO IOPT AT ',A8,1X,A8)
C
C**********************************************************************
C
C     TO CHECK FOR SUBSCRIPTS OVERRANGING, RUN UNDER IBM FORTRAN 4G AND
C     REMOVE THE 'C' FROM THE FOLLOWING 2 CARDS...
C     DEBUG SUBCHK
C     AT  2
      END
      SUBROUTINE STDIN
C
C     SUBROUTINE TO READ IN LIBRARY STANDARDS AND INFORMATION
C
      INTEGER TNAME,FM
      REAL*8 XIDT,TISO,TISOT
      DIMENSION YZ(256),A(22,22),Y(257),Z(22),CC(22),STD(22),B(22),
     $          R(256),W(256),DER(256),YT(256),IR(256),BA(256),FM(8),
     $          SS(20,4),AC(20,4),HA(20),IS(22),TST(22),HAT(22),AT(22),
```

```
     $          STDT(22),TNAME(20),TISOT(22),TISO(22),IT(22),ZT(22),
     $          S(20,256,4),XPF(20),XPET(20),YC(256),L1(3),YOBS(256)
      COMMON/STUFF/XIDT,TISOT,NS,M,NIT,NBA,NZ,MF,NH,KK,NTS,NTM,NQ,Q,FX,
     $          MS,NSAMP,NOPT,IPRINT,NBR,NBS,IABP,TB,TSA,VRED,DAY,VM,
     $          NBN,NB,NW,N,KT,LW,YOBS,K23D,QH,NDET,IS,MO,NRED,IN,FS,
     $         NBR1,FM,S,SS,AC,NDETS,HA,TST,Y,YC,IDPT,IAUX,R,XMOD,IRD,MU
C
C     GET DESCRIPTION OF GEOMETRY, # STDS., # DETECTORS
C
      READ(NTS) L1,NS,NDETS
      WRITE(MO,107) L1,NS,NDETS
C
C     GET NUCLIDES NAMES, HALFLIVES, COUNT TIMES, ACTIVITIES
C
      READ(NTS) (TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,NS)
      WRITE(MO,102)
      WRITE(MO,101) (TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,NS)
C
C     FOR EACH DETECTOR-GEOMETRY SET
C
      DO 50 K=1,NDETS
C
      DO 10 I=1,NS
C
C     READ SPECTRA FOR ALL NUCLIDES
C
      READ(NTS) TNAME
      IF (NBA.EQ.1) WRITE(MO,106) TNAME
      READ(NTS) (S(I,J,K),J=1,M)
      IF (NBA.EQ.1) WRITE(MO,103) (S(I,J,K),J=1,M)
10    CONTINUE
C
C     CALCULATE NUCLIDE CHANNEL SUMS
C
      DO 15 I=1,NS
      SS(I,K) = 0.0
      DO 15 J   NZ,MF
15    SS(I,K) = SS(I,K) + S(I,J,K)
C
C     CALCULATE NUCLIDE CHANNEL SUM SQUARES
C
      DO 20 I = 1,NS
20    SS(I,K) = SS(I,K)**2
C
50    CONTINUE
C
100   FORMAT(A8,6F10.2)
101   FORMAT(1X,A8,5X,F10.1,7X,F10.5,6X,F10.1,3X,F10.1,3X,F10.1,3X,F10.1
     $)
102   FORMAT(/,1X,'NUCLIDE',4X,'HALF-LIFE(DAYS)',3X,'CNT-TIME(MINS)',
     $3X,'ACT-DET-A',4X,'ACT-DET-B',4X,'ACT-DET-C',4X,'ACT-DET-D',/)
103   FORMAT(1X,10F12.1)
  106 FORMAT(1H1,20A4)
107   FORMAT('0FILE CONTAINS DATA FOR GEOMETRY TYPE ',3A4,10X,
     $'NUMBER OF STDS IS',I3,10X,'NUMBER OF DETECTORS IS',I3)
C
      RETURN
      END
      SUBROUTINE RESIDU
C
```

```
C      SUBROUTINE TO PROVIDE ANALYSIS OF RESIDUALS
C
       INTEGER LINE(101),NSTAR/'*'/,NBLNK/' '/,NPNT/'.'/,NPLUS/'+'/
       INTEGER TNAME,FM
       REAL*8 XIDT,TISO,TISOT
       DIMENSION YZ(256),A(22,22),Y(257),Z(22),CC(22),STD(22),B(22),
     $          R(256),W(256),DER(256),YT(256),IR(256),BA(256),FM(8),
     $          SS(20,4),AC(20,4),HA(20),IS(22),TST(22),HAT(22),AT(22),
     $          STDT(22),TNAME(20),TISOT(22),TISO(22),IT(22),ZT(22),
     $          S(20,256,4),XPE(20),XPET(20),YC(256),
     $          DA(22,22),ZUC(22),ZTUC(22),YOBS(256)
       COMMON/STUFF/XIDT,TISOT,NS,M,NIT,NBA,NZ,MF,NH,KK,NTS,NTM,NQ,Q,FX,
     $          MS,NSAMP,NOPT,IPRINT,NBR,NBS,IABP,TB,TSA,VRED,DAY,VM,
     $          NBN,NB,NW,N,KT,LW,YOBS,K23D,QH,NDET,IS,MO,NRED,IN,FS,
     $         NBRI,FM,S,SS,AC,NDETS,HA,TST,Y,YC,IOPT,IAUX,R,XMOD,IRD,MU
C
C      OUTPUT NORMALIZED RESIDUALS
C
       WRITE(MO,79)
       WRITE(MO,80)(R(J),J=1,MF)
       K = 0
       SIG3 = 0.
       SIG2 - 0.
       SIG1 = 0.
       SUMT - 0.
       XRSUM = 0
       XSQSUM = 0
       XCBSUM = 0
       X4TH = 0.
C
C      DETERMINE STATISTICS AND SUSPICIOUS CHANNELS FROM RESIDUALS
C
       DO 164  J = NZ,MF
       XRSUM - XRSUM + R(J)
       XSQSUM   XSQSUM + R(J)*R(J)
   164 XCBSUM = XCBSUM + R(J)*R(J)*R(J)
       XNO = MF-NZ + 1
       XAVG = XRSUM/XNO
       XSIG   SQRT((1./(XNO-1.))*(XSQSUM-((XRSUM**2)/XNO)))
       DO 163 J   NZ,MF
       SUMI - SUMI + ((R(J)-XAVG)/XSIG)**3
   163 SUMT - SUMT + ((R(J)-XAVG)/XSIG)**4
       XSKEW = SUMI/XNO
       XKURT = SUMT/XNO
       PLUS3S = XAVG + 3.0 * XSIG
       XMIN3S   XAVG - 3.0 * XSIG
       DO 165  J = NZ,MF
       IF ((R(J).LT.PLUS3S).AND.(R(J).GT.XMIN3S)) GO TO 165
       K = K + 1
       JCHNL = J
       IF (R(J).LT.XMIN3S) JCHNL   JCHNL * (-1)
   165 IR(K) = JCHNL
       WRITE(MO,84) XAVG,XSIG,XSKEW,XKURT
       DO 1655 J=NZ,MF
       IF ((R(J).LE.(3.*XSIG)).AND.(R(J).GE.(-3.*XSIG)))SIG3=SIG3+1.
       IF ((R(J).LE.(2.*XSIG)).AND.(R(J).GE.(-2.*XSIG)))SIG2=SIG2+1.
  1655 IF((R(J).LE.(XSIG)).AND.(R(J).GE.(-XSIG)))SIG1=SIG1+1.
       SIG3 = (SIG3/XNO) * 100.
       SIG2 = (SIG2/XNO) * 100.
       SIG1 = (SIG1/XNO) * 100.
```

```
      WRITE(MO,83) SIG1,SIG2,SIG3
      IF (K.EQ.0) GO TO 166
      WRITE(MO,81)
      WRITE(MO,82) (IR(J),J=1,K)
C
C     PRODUCE PRINT-PLOT OF NORMALIZED RESIDUALS
C
166   IF(IRD.EQ.0) GO TO 1000
      WRITE(MU,85) XIDT,IN
      WRITE(MU,88)
      N3P = (PLUS3S+10.0)/0.2
      N3M = (XMIN3S+10.0)/0.2
      IF (N3P.GT.101) N3P = 101
      IF (N3M.LT.1) N3M - 1
      DO 10 J   NZ,MF
      DO 5 K = 1,101
5     LINE(K) - NBLNK
      LINE(N3P) = NPNT
      LINE(N3M) = NPNT
      LINE(51) = NPNT
      NPOS - (R(J) + 10.0)/0.2 + 1
      IF (NPOS.GT.101) NPOS = 101
      IF (NPOS.LT.1) NPOS = 1
      LINE (NPOS) = NSTAR
10    WRITE(MU,500) J,R(J),NSTAR,LINE,NSTAR
C
C     PRODUCE PRINT-PLOT OF OBS'D AND CALC'D SPECTRA
C
      IF (IRD.NE.2) GO TO 1000
      YOFSET   0.0
      YMIN = 1.0E+20
      YMAX = -1.0E+20
      DO 15 I=NZ,MF
      IF (YOBS(I).GT.YMAX) YMAX   YOBS(I)
      IF (YC(I).GT.YMAX) YMAX = YC(I)
      IF (YOBS(I).LT.YMIN) YMIN = YOBS(I)
15    IF (YC(I).LT.YMIN) YMIN = YC(I)
      IF (YMIN) 16,17,17
16    YOFSET = ABS(YMIN)
17    YRANGE = YMAX - YMIN
      YINC = YRANGE/100.0
      WRITE(MU,86) XIDT,IN
      WRITE(MU,89)
      DO 25 I=NZ,MF
         DO 20 J=1,101
 20    LINE(J) = NBLNK
      IF (YMIN.LT.0.) LINE(IFIX(YOFSET/YINC)+1) = NPNT
      NPOS   (YOBS(I)-YMIN)/YINC + 1
      LINE(NPOS) - NSTAR
      NPOS = (YC(I)-YMIN)/YINC + 1
      L I NE(NPOS) = NPLUS
25    WRITE(MU,87) I,YOBS(I),YC(I),NSTAR,LINE,NSTAR
C
   79 FORMAT(/,' NORMALIZED RESIDUALS PER CHANNEL')
   80 FORMAT (1X,20F6.1)
   81 FORMAT (/,' SUSPICIOUS CHANNELS',/)
   82 FORMAT (25I5)
   83 FORMAT(1X,'PERCENT OF RESIDUALS UNDER 1 SIGMA =',F5.1,5X,
     $'2 SIGMA =',F5.1,5X,'3 SIGMA =',F5.1)
   84 FORMAT(/,1X,'AVERAGE =',F7.4,10X,'STD. DEV. =',F7.4,10X,
```

```
     $'SKEWNESS =',F9.4,10X,'KURTOSIS =',F9.4)
85    FORMAT(1H1,' PLOT OF RESIDUALS VERSUS CHANNEL NUMBER',10X,
     $'SAMPLE ID: ',A8,10X,'OPTION NUMBER',I3,//)
86    FORMAT(1H1,' PLOT OF YOBS AND YCALC',10X,
     $'SAMPLE ID: ',A8,10X,'OPTION NUMBER',I3,//)
87    FORMAT(I5,2F10.2,103A1)
   88 FORMAT(/,'  CHNL        R')
   89 FORMAT(/,'  CHNL    YOBS       YCALC')
500   FORMAT(I6,5X,F5.1,5X,A1,101A1,A1)
C
1000  RETURN
      END
      SUBROUTINE SHIFT (Y,M,SH,F,SHC)
C
C     E. SCHOENFIELD, MARCH 25, 1966
C
      DIMENSION Y(257),YC(257)
      Y(1)=0.0
      TE=SHC+SH*(F-1.0)
      JT=1
C
      DO 60  I=1,M
       QI=I
         DO 40  J=JT,M
         Z=J
         QJ=Z*F+TE
         IF (QI-QJ) 41,45,40
   41    IF ( J-1 ) 45,45,50
   45    YC(I)=Y(J)/F
         JT=J
         GO TO 60
   40    CONTINUE
   76 FORMAT(I6,6X,A8,4(4X,F9.4),7X,F6.2,4X,F9.4)
   50    YC(I)=(Y(J)-Y(J-1))/F
         YC(I)=Y(J-1)+YC(I)*(QI-QJ+F)
         YC(I)=YC(I)/F
         JT=J
   60 CONTINUE
      DO 80  I=1,M
   80 Y(I)=YC(I)
      YC(1)=1.0
      RETURN
      END
      SUBROUTINE INVERT (G,N,D)
C
C            GAUSS-JORDAN METHOD * VERSION BY
C            M H LIETZKE ET AL (ORNL-3430)
C
      DIMENSION A(22,22),B(22),C(22),LZ(22)
      DIMENSION  G (22,22)
      REAL * 8 A,B,C,W,Y,D,EPS
      EPS = 1.0D-10
      D = 1.0D0
      DO 40  I=1,N
       DO 41  J=1,N
       A(I,J)=G(I,J)
   41  CONTINUE
   40 CONTINUE
      DO 10  J=1,N
   10 LZ(J)=J
```

```
      DO 20 I=1,N
      K=I
      Y=A(I,I)
      L=I-1
      LP=I+1
      IF(N-LP)21,11,11
   11 DO 13 J=LP,N
      W=A(I,J)
      IF (DABS(W)-DABS(Y))13,13,12
   12 K=J
      Y=W
   13 CONTINUE
   21 IF (DABS(Y)-EPS) 24,24,25
   24 Y = 1.0
      WRITE (6,9923)
 9923  FORMAT (' ******** MATRIX IS SINGULAR *********')
   25 CONTINUE
   14 DO 15 J=1,N
      C(J)=A(J,K)
      A(J,K)=A(J,I)
      A(J,I)=-C(J)/Y
      A(I,J)=A(I,J)/Y
   15 B(J)=A(I,J)
      A(I,I)=1.0D+0/Y
      J=LZ(I)
      LZ(I)=LZ(K)
      LZ(K)=J
      DO 19 K=1,N
      IF(I-K)16,19,16
   16 DO 18 J=1,N
      IF(I-J)17,18,17
   17 A(K,J)=A(K,J)-B(J)*C(K)
   18 CONTINUE
   19 CONTINUE
   20 CONTINUE
      DO 200 I=1,N
      IF(I-LZ(I))100,200,100
  100 K=I+1
      IF(I-N)800,200,200
  800 DO 500 J=K,N
      IF(I-LZ(J))500,600,500
  600 M=LZ(I)
      LZ(I)=LZ(J)
      LZ(J)=M
      DO 700 L=1,N
      C(L)=A(I,L)
      A(I,L)=A(J,L)
  700 A(J,L)=C(L)
  500 CONTINUE
  200 CONTINUE
      DO 42 I=1,N
       DO 43 J=1,N
       G(I,J)=A(I,J)
   43  CONTINUE
   42 CONTINUE
      RETURN
      END
      SUBROUTINE LABEL
C
C     SUBROUTINE TO PROVIDE LABELS FOR INPUT PARAMETERS
```

```
C
      INTEGER TNAME,FM
      REAL*8 XIDT,TISO,TISOT
      DIMENSION YZ(256),A(22,22),Y(257),Z(22),CC(22),STD(22),B(22),
     $          R(256),W(256),DER(256),YT(256),IR(256),BA(256),FM(8),
     $          SS(20,4),AC(20,4),HA(20),IS(22),TST(22),HAT(22),AT(22),
     $          STDT(22),TNAME(20),TISOT(22),TISO(22),IT(22),ZT(22),
     $          S(20,256,4),XPE(20),XPET(20),YC(256),YOBS(256)
      COMMON/STUFF/XIDT,TISOT,MS,M,NIT,NBA,NZ,MF,NH,KK,NTS,NTM,NQ,Q,FX,
     $          MS,NSAMP,NOPT,IPRINT,NBR,NBS,IABP,TB,TSA,VRED,DAY,VM,
     $          NBN,NB,NW,N,KT,LW,YOBS,K23D,QH,NDET,IS,MO,NRED,IN,FS,
     $         NBR1,FM,S,SS,AC,NDETS,HA,TST,Y,YC,IOPT,IAUX,R,XMOD,IRD,MU
C
C     LABEL GENERAL CONTROL INFORMATION
C
      WRITE(MO,1) FM,M,NIT,NZ,MF,NTS,NTM
      IF (NBA.GT.0) GO TO 100
      WRITE(MO,2)
      GO TO 110
100   WRITE(MO,3)
110   IF (NH.GT.0) GO TO 115
      WRITE(MO,36)
      GO TO 117
115   WRITE(MO,35)
117   IF (IAUX.EQ.0) GO TO 118
      WRITE(MO,38) IAUX
      GO TO 119
118   WRITE(MO,39)
119   IF (IOPT.EQ.0) GO TO 120
      WRITE(MO,40) IOPT
      GO TO 121
120   WRITE(MO,41)
121   IF (MS.GT.0) GO TO 122
      WRITE(MO,43)
      GO TO 123
122   WRITE(MO,42) MU
123   RETURN
C
C     LABEL SAMPLE CONTROL INFORMATION
C
      ENTRY LABEL1
      NSMP   NRED + 1
      WRITE(MO,4) NSMP,XIDT,NOPT,TB,TSA,DAY,VRED,VM,FS,FX
130   IF (NBR.GT.0) GO TO 140
      WRITE(MO,7)
      GO TO 150
140   WRITE(MO,8)
150   IF (NBS.GT.0) GO TO 160
      WRITE(MO,9)
      GO TO 170
160   WRITE(MO,10)
170   GO TO (171,172,173,174),IABP
171   WRITE(MO,11)
      GO TO 175
172   WRITE(MO,12)
      GO TO 175
173   WRITE(MO,13)
      GO TO 175
174   WRITE(MO,14)
175   IF (MS.EQ.0) GO TO 176
```

```
      WRITE(MO,44) MS
176   RETURN
C
C     LABEL SAMPLE OPTION INFORMATION
C
      ENTRY LABEL2
      WRITE(MO,33) NRED,XIOT,IN
      IF (NB.GT.0) GO TO 220
      WRITE(MO,15)
      GO TO 230
220   WRITE(MO,16)
230   IF (NW.GT.0) GO TO 240
      WRITE(MO,17)
      GO TO 250
240   WRITE(MO,18)
250   IF (IABS(NW)-2) 260,270,280
260   WRITE(MO,19)
      GO TO 290
270   WRITE(MO,20)
      GO TO 290
280   WRITE(MO,21)
290   IF (Q.GT.0) GO TO 300
      WRITE(MO,22)
      GO TO 310
300   IF (KK.EQ.0) GO TO 305
      WRITE(MO,34) Q
      GO TO 310
305   WRITE(MO,23) Q
310   NEKT = KT+3
      GO TO (320,330,340,350,350), NEKT
320   WRITE(MO,24)
      GO TO 360
330   WRITE(MO,25)
      GO TO 360
340   WRITE(MO,26)
      GO TO 360
350   WRITE(MO,27)
360   IF (KT.LT.0) GO TO 380
      IF (KT.EQ.1) GO TO 370
      WRITE(MO,28)
      GO TO 380
370   WRITE(MO,29)
380   WRITE(MO,30) N
      WRITE(MO,31) QH
      WRITE(MO,32) (IS(I),I=1,N)
      IF (XMOD) 390,395,390
390   WRITE(MO,45) XMOD
395   IF (IRD.GT.0) GO TO 400
      WRITE(MO,47)
      GO TO 405
400   WRITE(MO,46)
405   IF (IRD.EQ.2) GO TO 407
      WRITE(MO,50)
      GO TO 408
407   WRITE(MO,51)
408   IF (IPRINT.EQ.0) GO TO 410
      WRITE(MO,49)
      GO TO 415
410   WRITE(MO,48)
415   WRITE(MO,37)
```

```
      RETURN
C
1     FORMAT(1H0,'GENERAL CONTROL INFORMATION ',//,
     $        1X,'DATA FORMAT IS ',8A4,/,
     $        1X,'NUMBER OF CHANNELS IN ANALYZER IS',I5,/,
     $        1X,'MAXIMUM NUMBER OF ITERATIONS IS',I3,/,
     $        1X,'INITIAL CHANNEL FOR COMPUTATION IS',I4,/,
     $        1X,'FINAL CHANNEL FOR COMPUTATION IS',I4,/,
     $        1X,'STANDARD SPECTRA ON FORTRAN LOGICAL UNIT',I3,/,
     $        1X,'SAMPLE SPECTRA ON FORTRAN LOGICAL UNIT',I3)
2     FORMAT(1X,'LIBRARY STANDARD SPECTRA WILL NOT BE PRINTED')
3     FORMAT(1X,'LIBRARY STANDARD SPECTRA WILL BE PRINTED')
4     FORMAT(1H1,'CONTROL INFORMATION ..... SAMPLE NUMBER',I3,
     $        10X,'SAMPLE ID IS: ',A8,/,/,
     $        1X,'NUMBER OF PROCESSING OPTIONS IS',I3,/,
     $        1X,'COUNTING TIME (MINS.) FOR BKGND IS',F8.2,/,
     $        1X,'COUNTING TIME (MINS.) FOR SAMPLE IS',F8.2,/,
     $        1X,'DECAY TIME (DAYS) IS',F7.2,/,
     $        1X,'VOLUME REDUCTION FACTOR IS',F7.3,/,
     $        1X,'VOLUME MULTIPLICATION FACTOR IS',F7.3,/,
     $        1X,'SAMPLE TIME/BKGND TIME = FS =',F7.3,/,
     $        1X,'VALUE OF FS**2 = FX =',F7.3)
    7 FORMAT (1X,'SAMPLE BACKGROUND NOT INPUT; PREVIOUS BKGND WILL BE US
     $ED IF SUBTRACTION REQUESTED')
8     FORMAT (1X,'SAMPLE BACKGROUND WILL BE INPUT AND USED IF SUBTRACTIO
     $N REQUESTED')
9     FORMAT (1X,'PERMANENT BACKGROUND SUBTRACTION NOT REQUESTED')
10    FORMAT (1X,'PERMANENT BACKGROUND SUBTRACTION REQUESTED')
11    FORMAT (1X,'DETECTOR A STANDARDS SELECTED',/)
12    FORMAT (1X,'DETECTOR B STANDARDS SELECTED',/)
13    FORMAT(1X,'DETECTOR C STANDARDS SELECTED',/)
14    FORMAT(1X,'DETECTOR D STANDARDS SELECTED',/)
15    FORMAT (1X,'BACKGROUND WILL NOT BE SUBTRACTED THIS OPTION')
16    FORMAT(1X,'BACKGROUND WILL BE SUBTRACTED THIS OPTION')
17    FORMAT (1X,'WEIGHTS TO BE BASED ON OBSERVED SAMPLE SPECTRUM')
18    FORMAT(1X,'WEIGHTS TO BE BASED ON CALCULATED SAMPLE SPECTRUM')
19    FORMAT(1X,'WEIGHTS PROPORTIONAL TO RECIPROCAL COUNTS/CHANNEL')
20    FORMAT(1X,'WEIGHTS PROPORTIONAL TO RECIPROCAL VARIANCE OF COUNTS/C
     $HANNEL')
21    FORMAT(1X,'UNIT WEIGHTS ASSUMED')
22    FORMAT(1X,'NO REJECTION COEFFICIENT APPLIED')
23    FORMAT(1X,'REJECTION COEFFICIENT OF ',F6.2,' WILL BE APPLIED')
24    FORMAT(1X,'COMPENSATION BASED ON PREVIOUSLY CALCULATED VALUES')
25    FORMAT(1X,'MANUAL COMPENSATION REQUIRED')
26    FORMAT(1X,'NO COMPENSATION REQUIRED')
27    FOPMAT(1X,'AUTOMATIC COMPENSATION REQUIRED')
28    FORMAT(1H+,T34,'FOR GAIN AND THRESHOLD SHIFT')
29     FORMAT(1H+,T34,'FOR GAIN SHIFT ONLY')
30    FORMAT(1X,'NUMBER OF ISOTOPES USED FROM LIBRARY IS',I3)
   31 FORMAT (1X,'THRESHOLD CHANNEL SHIFT BETWEEN STDS AND SAMPLE IS',
     $F6.2)
32    FORMAT(1X,'LIBRARY STD. NUMBERS, IN ORDER OF DESIRED OUTPUT ARE',
     $ 20I3)
33    FORMAT (1H1,'SAMPLE NUMBER',I3,'    ID NO. ',A8,' ... PROCESSING O
     $PTION NUMBER',I3,//)
34    FORMAT (1X,'REJECTION COEFFICIENT OF ',F6.2,' HAS BEEN APPLIED')
35    FORMAT (1X,'CORRELATIONS BETWEEN VARIABLES WILL BE PRINTED')
36    FORMAT (1X,'CORRELATIONS BETWEEN VARIABLES WILL NOT BE PRINTED')
37    FORMAT (/)
38    FORMAT(1X,'AUXILIARY DATA OUTPUT ON FORTRAN LOGICAL UNIT',I3)
```

```
39    FORMAT(1X,'AUXILIARY DATA WILL NOT BE OUTPUT')
40    FORMAT(1X,'ANALYTICAL RESULTS OUTPUT ON FORTRAN LOGICAL UNIT',I3)
41    FORMAT(1X,'ANALYTICAL RESULTS WILL NOT BE OUTPUT TO DISK')
42    FORMAT(1X,'FORTRAN LOGICAL UNIT FOR PRINT-PLOTS (IF REQUESTED) IS
     $',I3)
43    FORMAT(1X,'FORTRAN LOGICAL UNIT FOR PRINT-PLOTS NOT SUPPLIED')
44    FORMAT(1X,'LIBRARY STD. NO. ',I2,' BEING REPLACED WITH BKGND')
45    FORMAT(1X,30('*'),'  WEIGHTING MODIFICATION ',F6.2,3X,30('*'))
46    FORMAT(1X,'NORMALIZED RESIDUALS WILL BE PLOTTED')
47    FORMAT(1X,'NORMALIZED RESIDUALS WILL NOT BE PLOTTED')
48    FORMAT(1X,'MATRIX INFORMATION WILL NOT BE PRINTED')
49    FORMAT(1X,'MATRIX INFORMATION WILL BE PRINTED')
50    FORMAT(1X,'OBSERVED AND CALCULATED SPECTRA WILL NOT BE PLOTTED')
51    FORMAT(1X,'OBSERVED AND CALCULATED SPECTRA WILL BE PLOTTED')
C
      END
      SUBROUTINE DIAG
C
C     SUBROUTINE TO PROVIDE DIAGNOSTICS FOR INPUT PARAMETERS
C     SETS IER = 1 FOR TERMINAL ERROR
C
      REAL * 8 TISOT,TISO,XIDT,ADATE,ANOUN,D
      INTEGER * 4 FM,TNAME
      DIMENSION YZ(256),A(22,22),Y(257),Z(22),CC(22),STD(22),B(22),
     $          R(256),W(256),DER(256),YT(256),IR(256),BA(256),FM(8),
     $          SS(20,4),AC(20,4),HA(20),IS(22),TST(22),HAT(22),AT(22),
     $          STDT(22),TNAME(20),TISOT(22),TISO(22),IT(22),ZT(22),
     $          S(20,256,4),XPE(20),XPET(20),YC(256),XI(22,22),
     $          DA(22,22),ZUC(22),ZTUC(22),YOBS(256)
      COMMON/STUFF/XIDT,TISOT,NS,M,NIT,NBA,NZ,MF,NH,KK,NTS,NTM,NQ,Q,FX,
     $          MS,NSAMP,NOPT,IPRINT,NER,NBS,IABP,TB,TSA,VRED,DAY,VM,
     $          NBN,NB,NW,N,KT,LW,YOBS,K23D,QH,NDET,IS,MO,NRED,IN,FS,
     $          NBR1,FM,S,SS,AC,NDETS,HA,TST,Y,YC,IOPT,IAUX,R,XMOD,IRD,MU
      INTEGER ERROR(4) /'*****','** ER','ROR ','*****'/
C
C     DIAGNOSTICS FOR GENERAL CONTROL CARD
C
      IER = 0
      IF (M.LE.256) GO TO 100
      WRITE(MO,1) ERROR
1     FORMAT(4A4,5X,'NUMBER OF CHANNELS (M) GREATER THAN 256')
      IER - 1
100   IF (MF.LE.M) GO TO 110
      WRITE(MO,2) ERROR
2     FORMAT(4A4,5X,'FINAL CHANNEL (MF) GREATER THAN VALUE OF M')
      IER = 1
110   IF (MF.LE.256) GO TO 120
      WRITE(MO,3) ERROR
3     FORMAT(4A4,5X,'FINAL CHANNEL (MF) GREATER THAN 256')
      IER = 1
120   IF (NZ.LT.MF) GO TO 130
      WRITE(MO,4) ERROR
4     FORMAT(4A4,5X,'INITIAL CHANNEL (NZ) GREATER THAN FINAL (MF)')
      IER = 1
130   IF (NZ.GT.0) GO TO 140
      WRITE(MO,5) ERROR
5     FORMAT(4A4,5X,'INITIAL CHANNEL (NZ) IS ZERO OR LESS')
      IER = 1
140   IF (NTS.GT.0) GO TO 150
      WRITE(MO,6) ERROR
```

```
6       FORMAT(4A4,5X,'NO FORTRAN UNIT FOR STANDARD LIBRARY SPECTRA')
        IER    1
150     IF (NTM.GT.0) GO TO 160
        WRITE(MO,7) ERROR
7       FORMAT(4A4,5X,'NO FORTRAN UNIT FOR SAMPLE SPECTRA')
        IER = 1
160     IF (IER.EQ.0) RETURN
        WRITE(MO,8)
8       FORMAT('0JOB TERMINATED FOR ABOVE ERROR(S)')
        STOP 5095
C
C       DIAGNOSTICS FOR SAMPLE CONTROL CARD
C
        ENTRY DIAG1
        IER = 0
        IF ((NBS.EQ.1).AND.((NBR+NBR1).EQ.0)) GO TO 170
        GO TO 180
170     WRITE(MO,9) ERROR
9       FORMAT(4A4,5X,'BKGND SUBTRACTION REQUESTED BUT NO BKGND INPUT')
        IER    1
180     IF (IABP.LE.NDETS) GO TO 190
        WRITE(MO,10) ERROR
10      FORMAT(4A4,5X,'DETECTOR NO. IABP GREATER THAN ANY IN LIBRARY')
        IER = 1
190     IF (TB.GT.0.) GO TO 200
        WRITE(MO,11) ERROR
11      FORMAT(4A4,5X,'SAMPLE COUNT TIME IS ZERO MINUTES')
        IER = 1
200     IF ((TSA.LE.0.).AND.((NBR+NBR1).GT.0.)) GO TO 210
        GO TO 212
210     WRITE(MO,12) ERROR
12      FORMAT(4A4,5X,'BKGND COUNT TIME IS ZERO MINUTES')
        IER = 1
212     IF ((MS.GT.0).AND.((NBR+NBR1).EQ.0)) GO TO 215
        GO TO 220
215     WRITE(MO,18) ERROR
18      FORMAT(4A4,5X,'LIB. STD. REPLACEMENT REQUESTED BUT NO BKGND',
       $' SPECTRUM HAS BEEN INPUT')
        IER    1
220     IF (IER.EQ.0) RETURN
        WRITE(MO,8)
        STOP 5095
C
C       DIAGNOSTICS FOR SAMPLE OPTION CARD
C
        ENTRY DIAG2
        IER    0
        IF (N.LE.NS) GO TO 230
        WRITE(MO,13) ERROR
13      FORMAT(4A4,5X,'NO. NUCLIDES SELECTED IS GREATER THAN NO. IN',
       $' LIBRARY')
        IER = 1
230     IF ((NB.EQ.1).AND.((NBR+NBR1).EQ.0)) GO TO 240
        GO TO 250
240     WRITE(MO,14) ERROR
14      FORMAT(4A4,5X,'BKGND SUBTRACTION REQUESTED BUT NO BKGND INPUT')
        IER = 1
250     IF ((IABS(NW).EQ.2).AND.((NBR+NBR1).EQ.0)) GO TO 260
        GO TO 270
260     WRITE(MO,15) ERROR
```

```
15     FORMAT(4A4,5X,'WEIGHTING SCHEME SELECTED REQUIRES A BKGND',
      $' BUT NONE HAS BEEN INPUT')
       IER = 1
270    IF (N.GT.NS) GO TO 280
       IF1 - 0
       DO 272 INT = 1,N
       IF (IS(INT).LE.0) IF1 = 1
272    IF (IS(INT).GT.NS) IF1 = 1
       IF (IF1.EQ.1) GO TO 275
       GO TO 280
275    WRITE(MO,16) ERROR
16     FORMAT(4A4,5X,'ONE OR MORE LIB. STD. NOS. SELECTED ARE OUT',
      $' OF RANGE')
       IER = 1
280    NEND = N-1
       IF1 = 0
       DO 285 I = 1,NEND
       K = I+1
       DO 285 J = K,N
       IF (IS(I).EQ.IS(J)) IF1 - 1
285    CONTINUE
       IF (IF1.EQ.1) GO TO 290
       GO TO 295
290    WRITE(MO,17) ERROR
17     FORMAT(4A4,5X,'TWO OR MORE LIB. STDS SELECTED ARE REDUNDANT')
       IER = 1
295    IF (IER.EQ.0) RETURN
       WRITE(MO,8)
       STOP 5095
C
       END
```

A.6 ALPHA-M FLOW DIAGRAMS

The following figures are the flow diagrams for the computer program ALPHA-M. Figure A-1 (4 sheets) is the main program flow diagram, A-2 (5 sheets) is for the subroutine LABEL, A-3 is for the subroutine STDIN, A-4 is for the subroutine RESIDU, and A-5 (2 sheets) is for the subroutine DIAG.

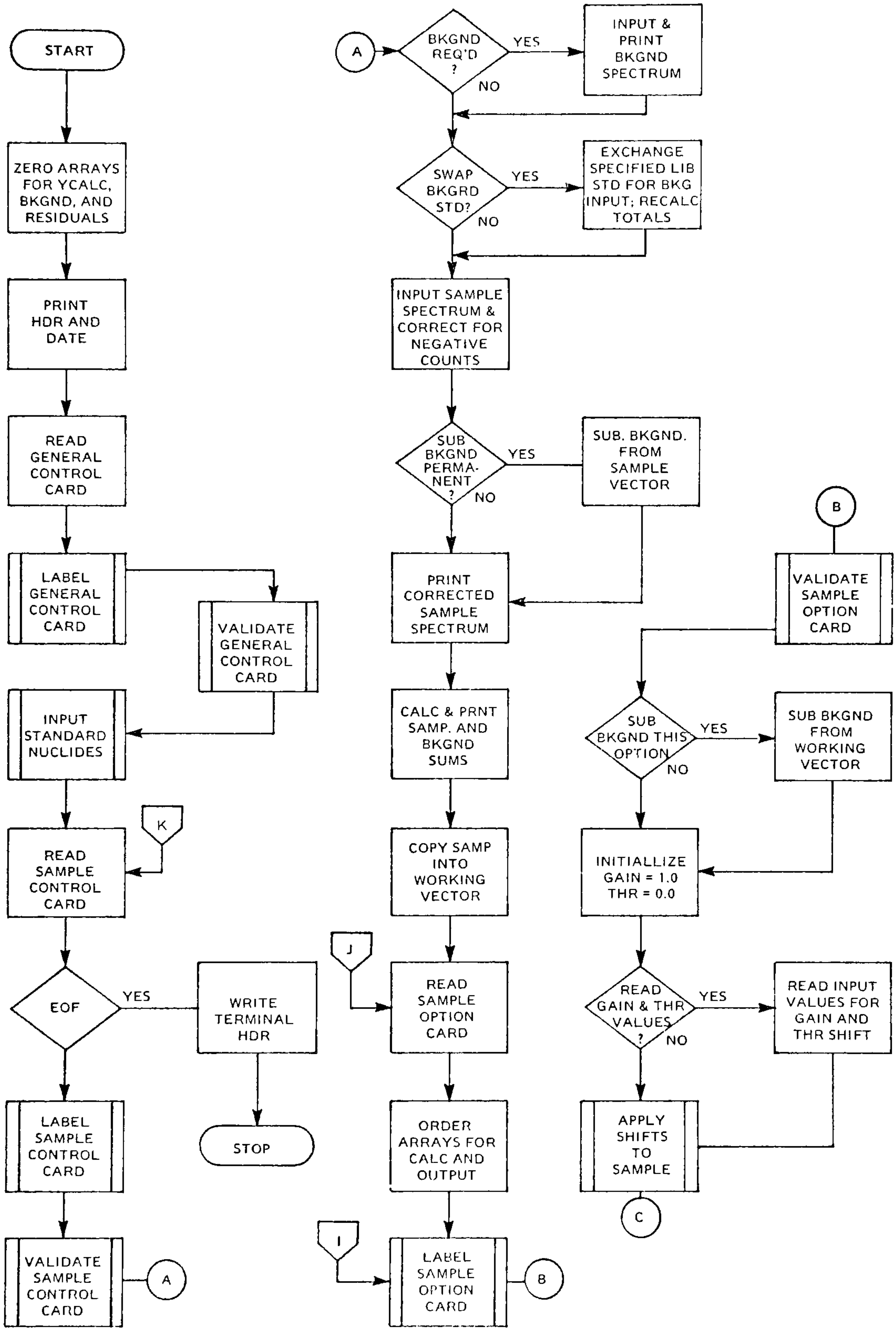

Figure A-1. ALPHA-M main program flow diagram.

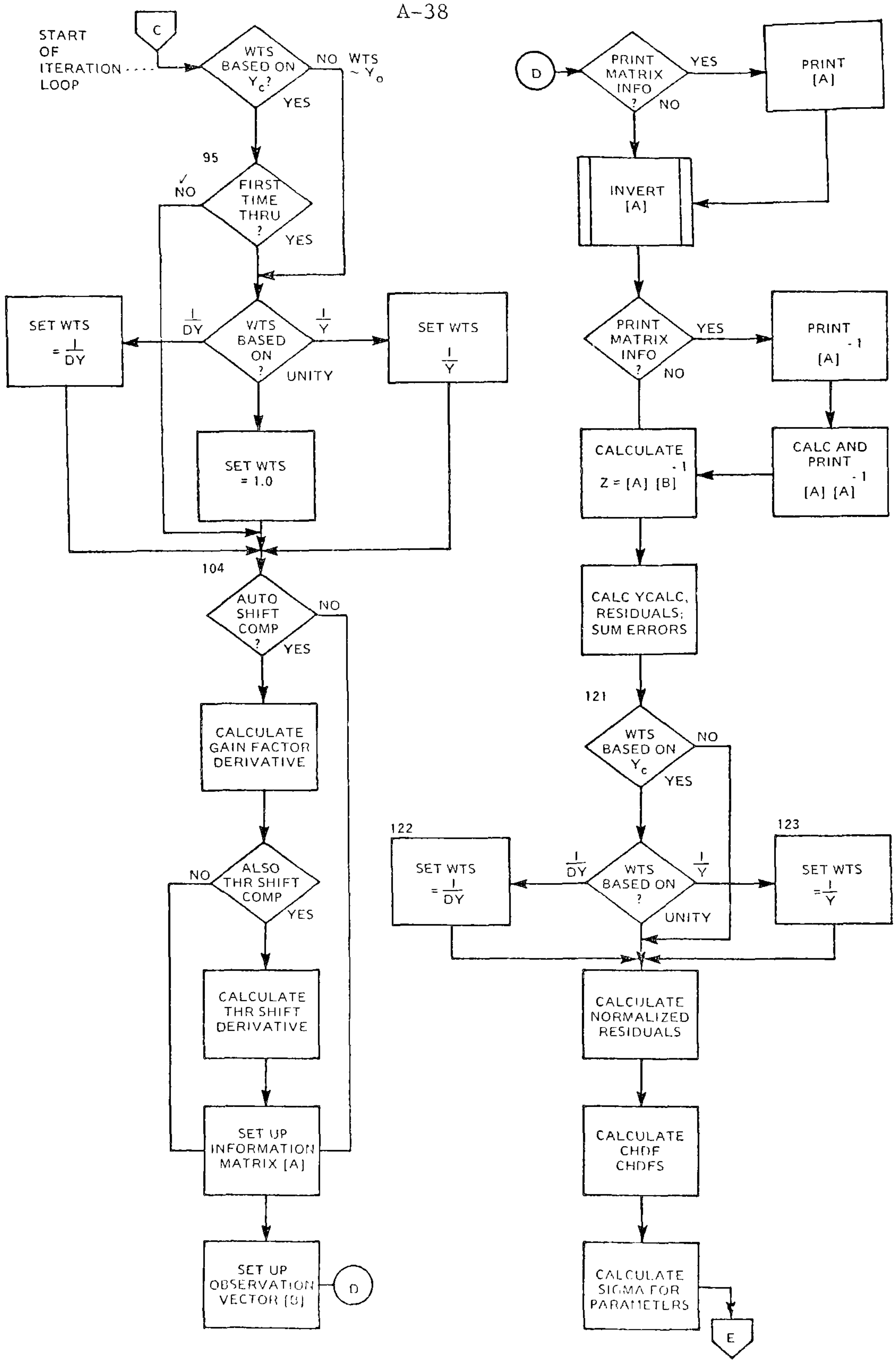

Figure A-1. ALPHA-M main program flow diagram (cont.)

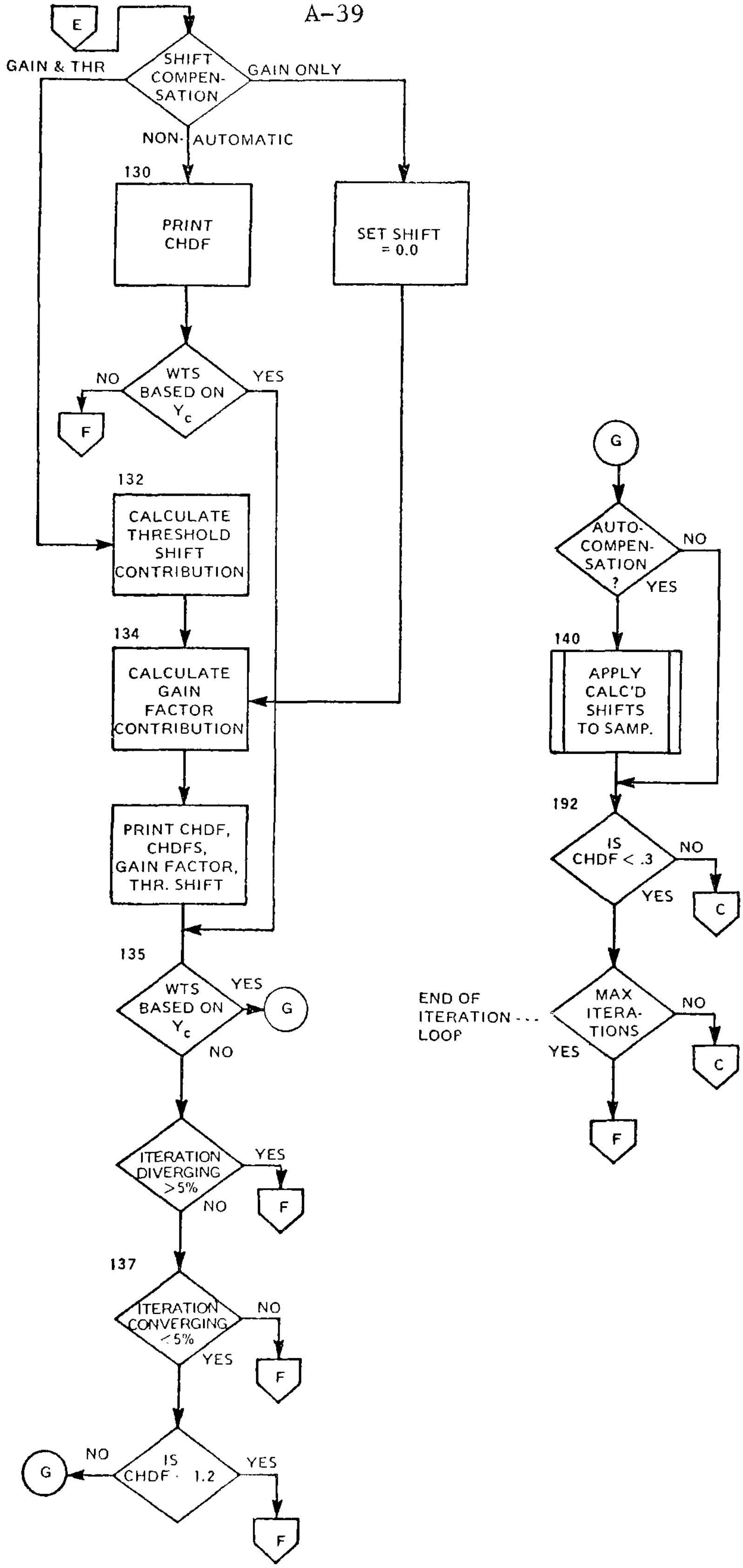

Figure A-1. ALPHA-M main program flow diagram (cont.)

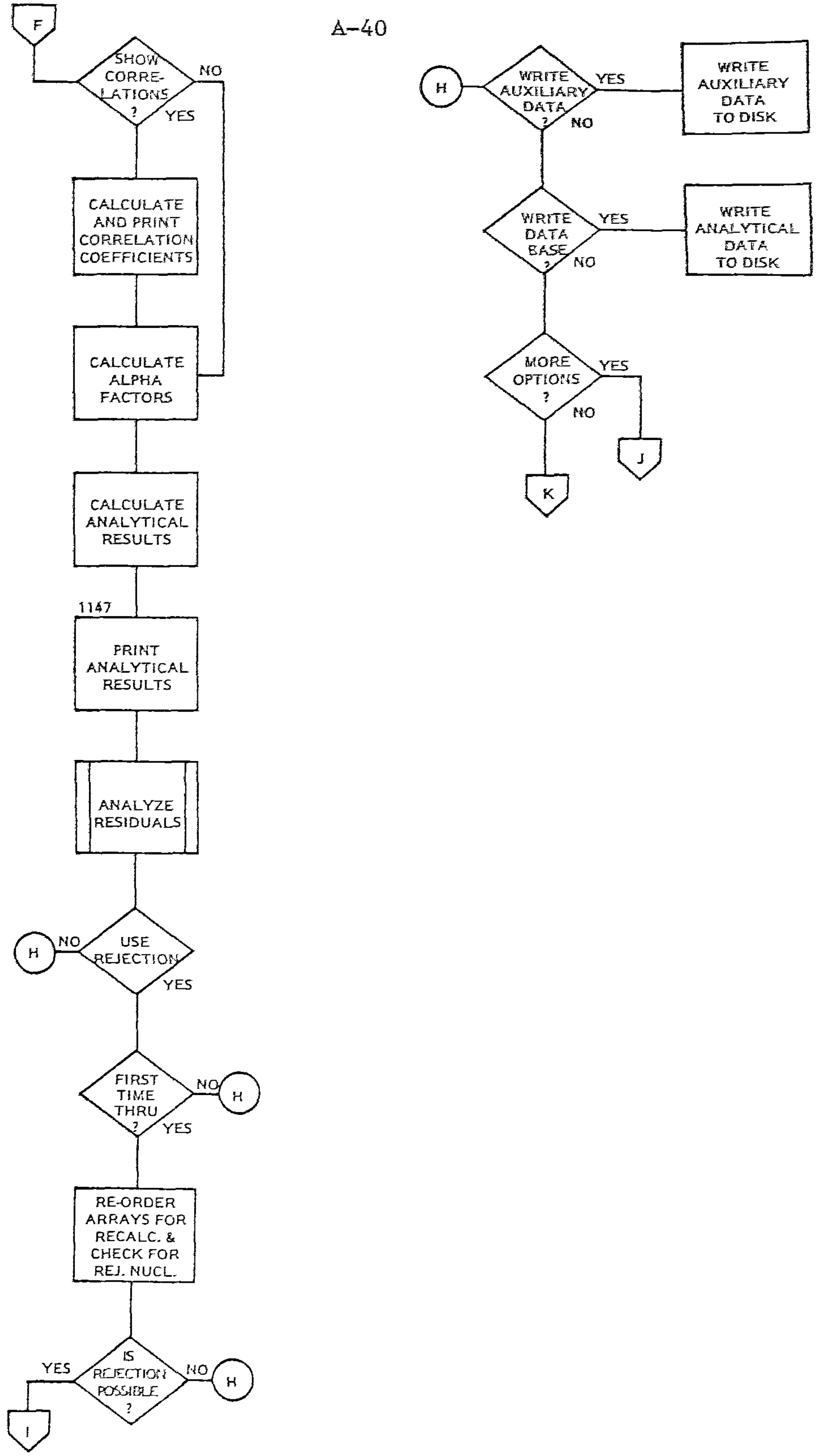

Figure A-1. ALPHA-M main program flow diagram (cont.)

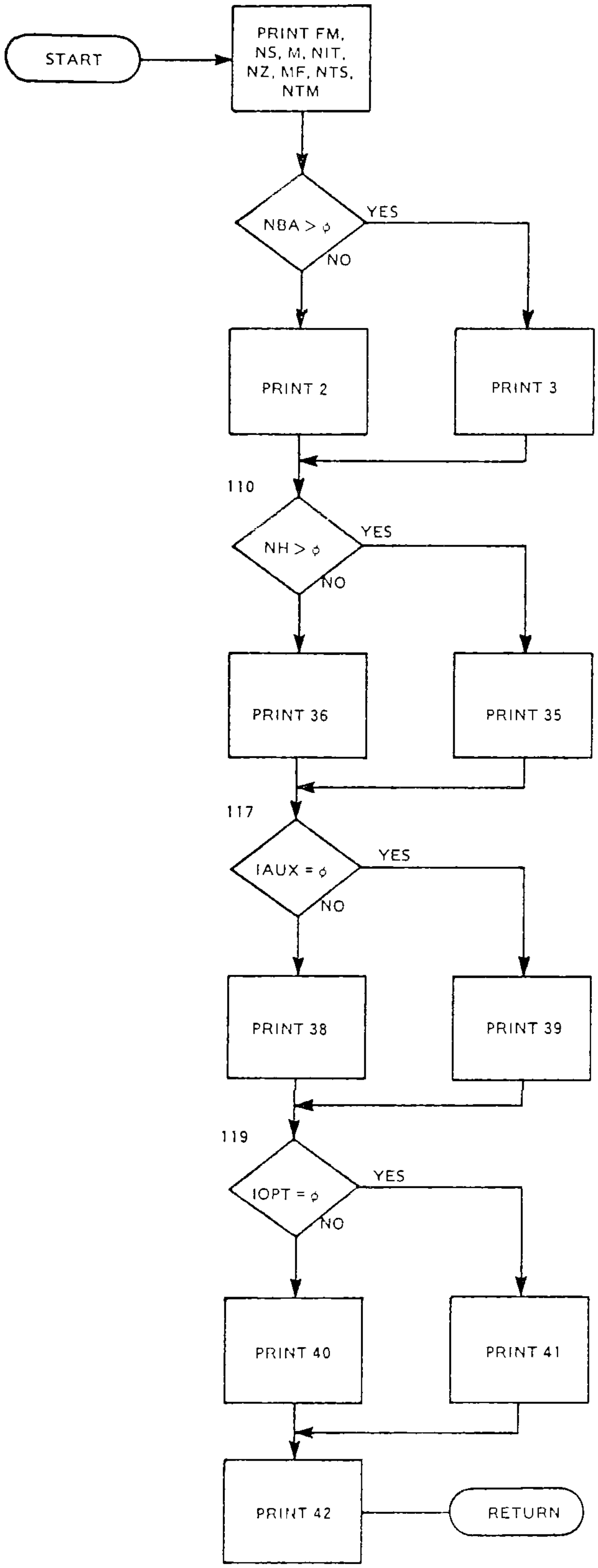

Figure A-2. ALPHA-M subroutine LABEL flow diagram.

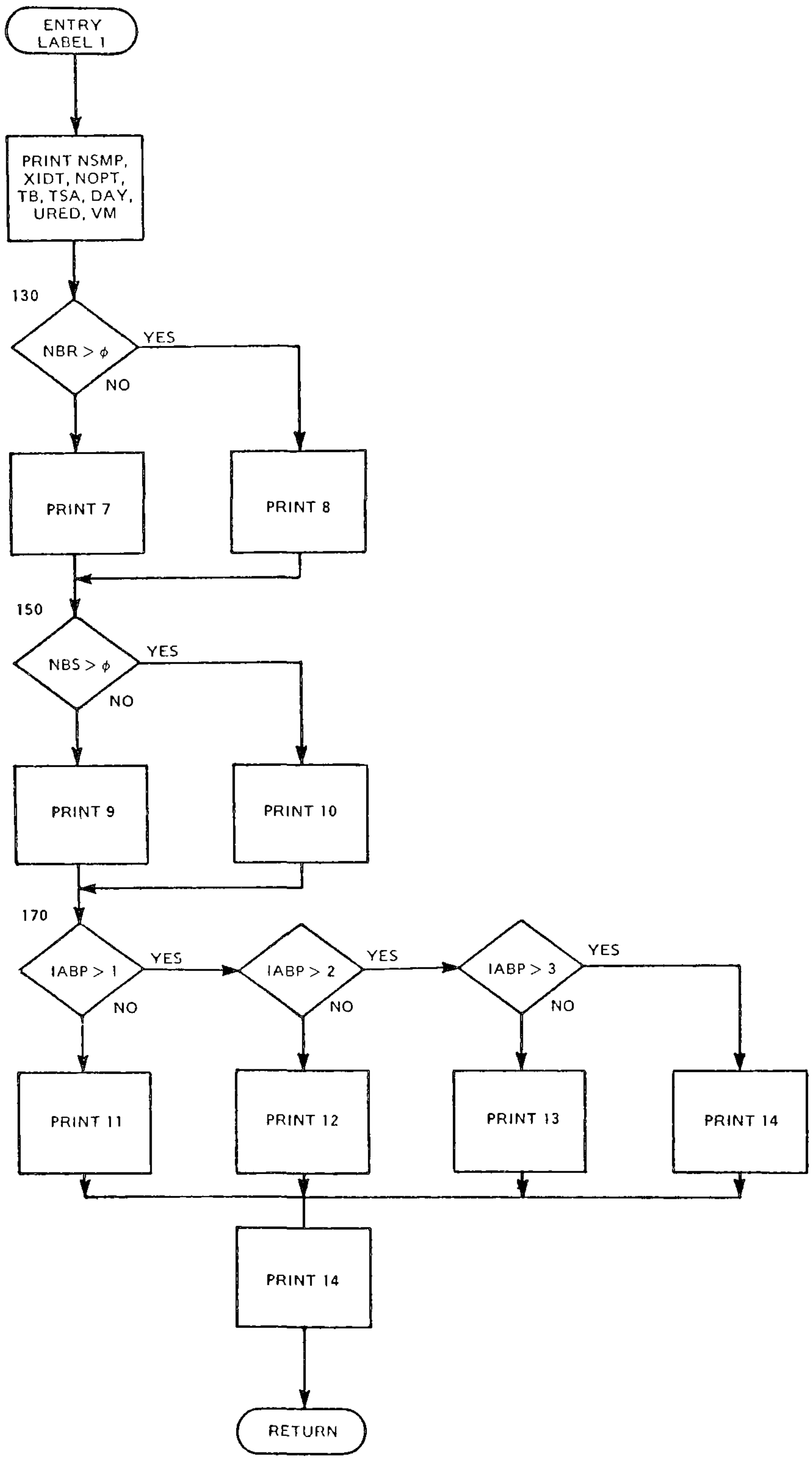

Figure A-2. ALPHA-M subroutine LABEL flow diagram (cont.)

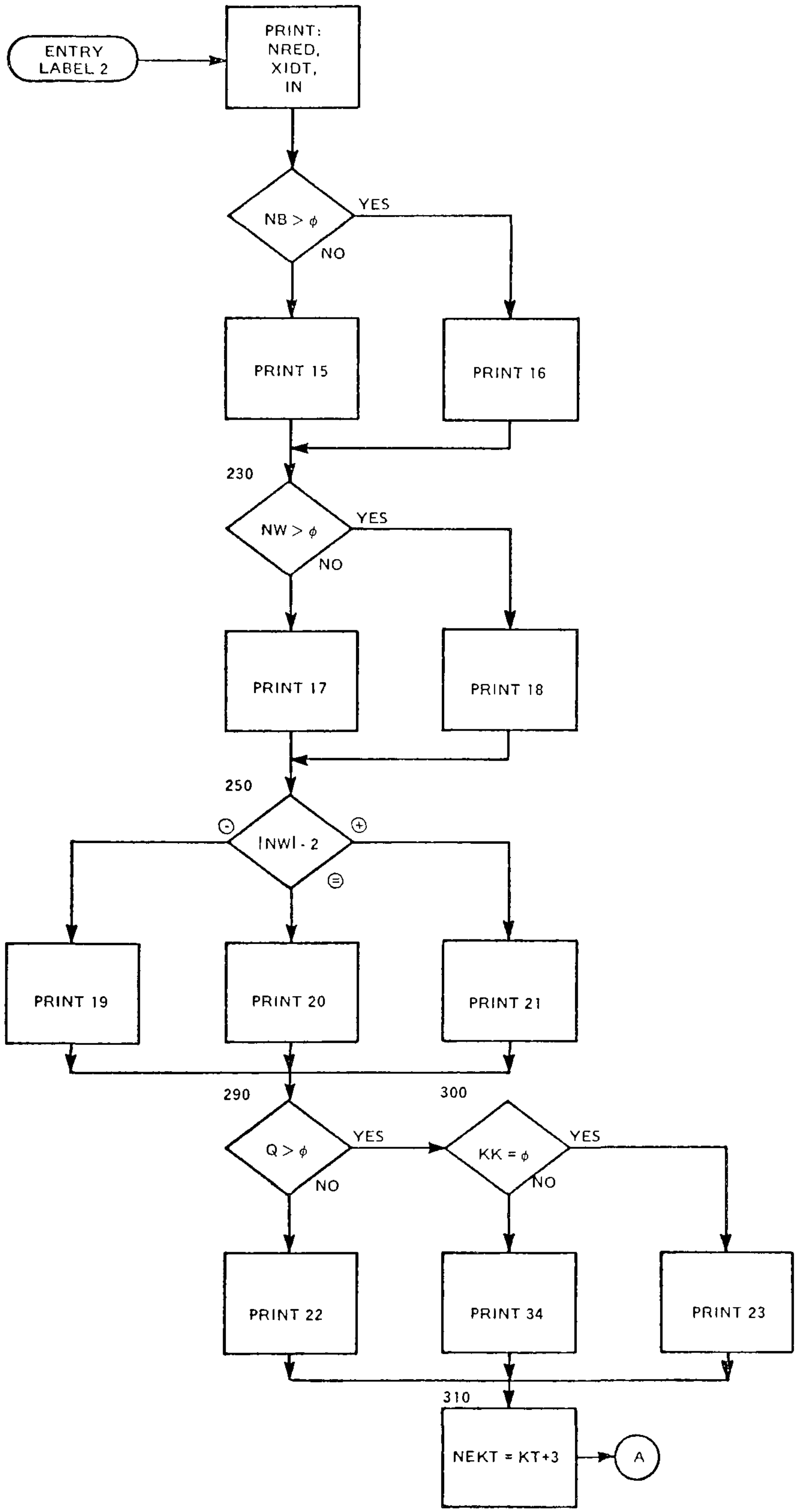

Figure A-2. ALPHA-M subroutine LABEL flow diagram (cont.)

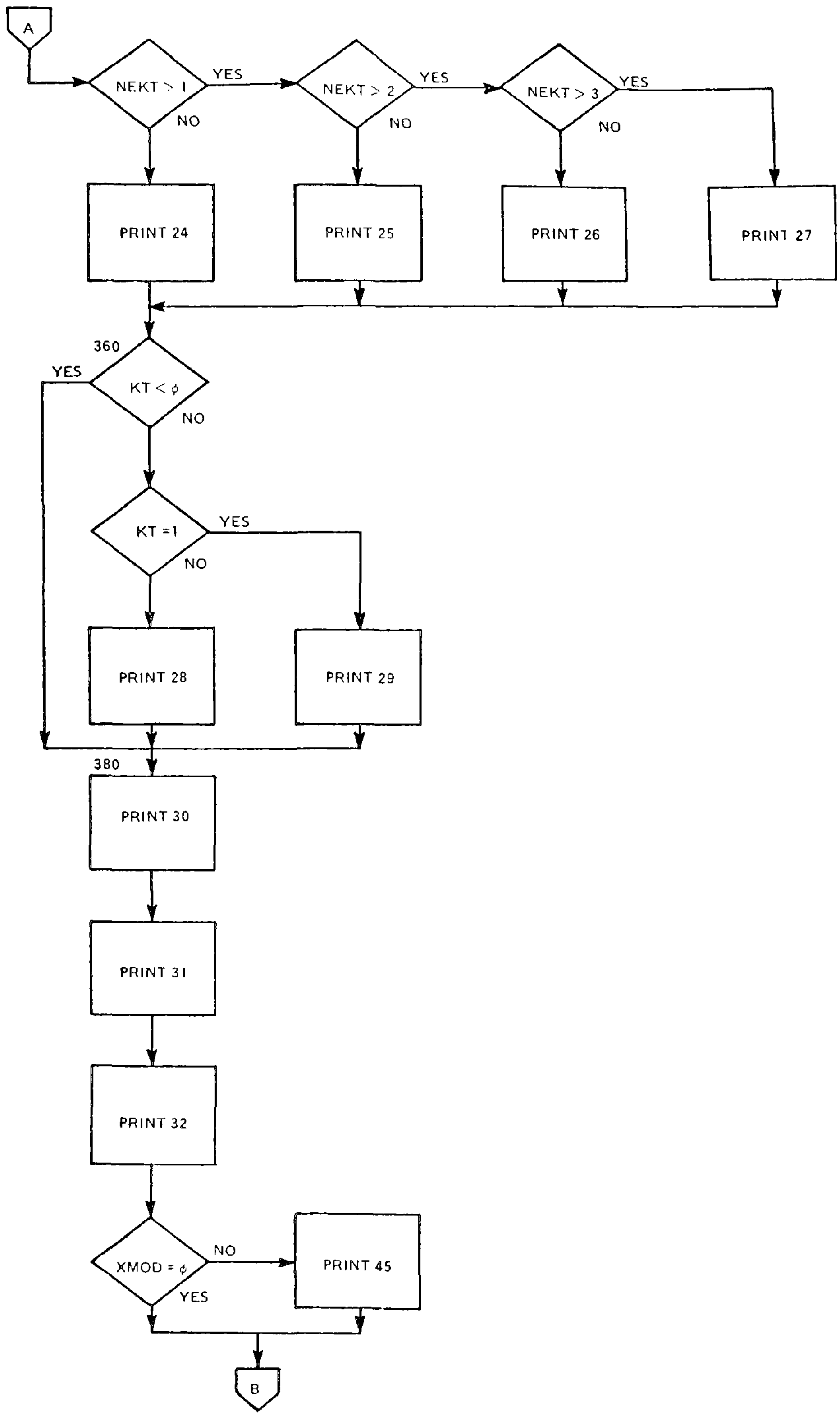

Figure A-2. ALPHA-M subroutine LABEL flow diagram (cont.)

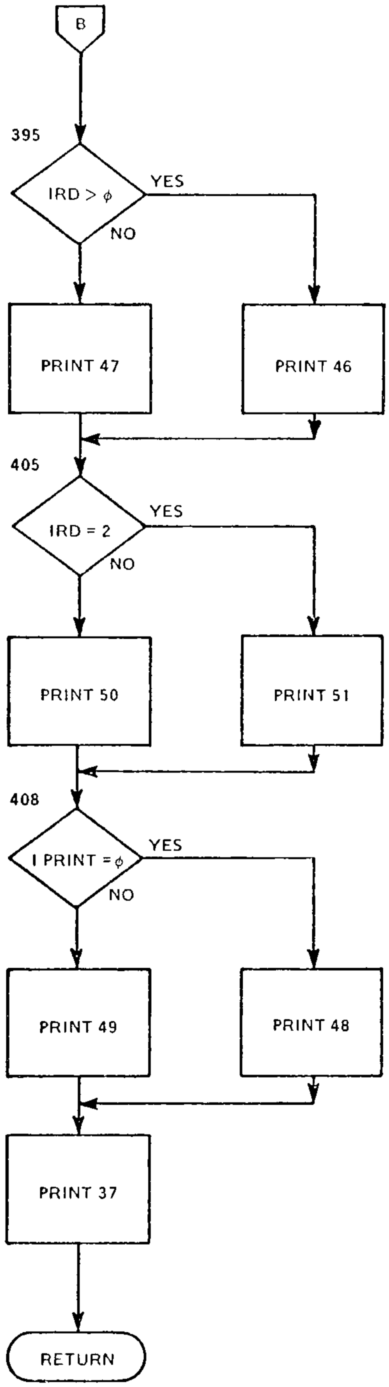

Figure A-2. ALPHA-M subroutine LABEL flow diagram (cont.)

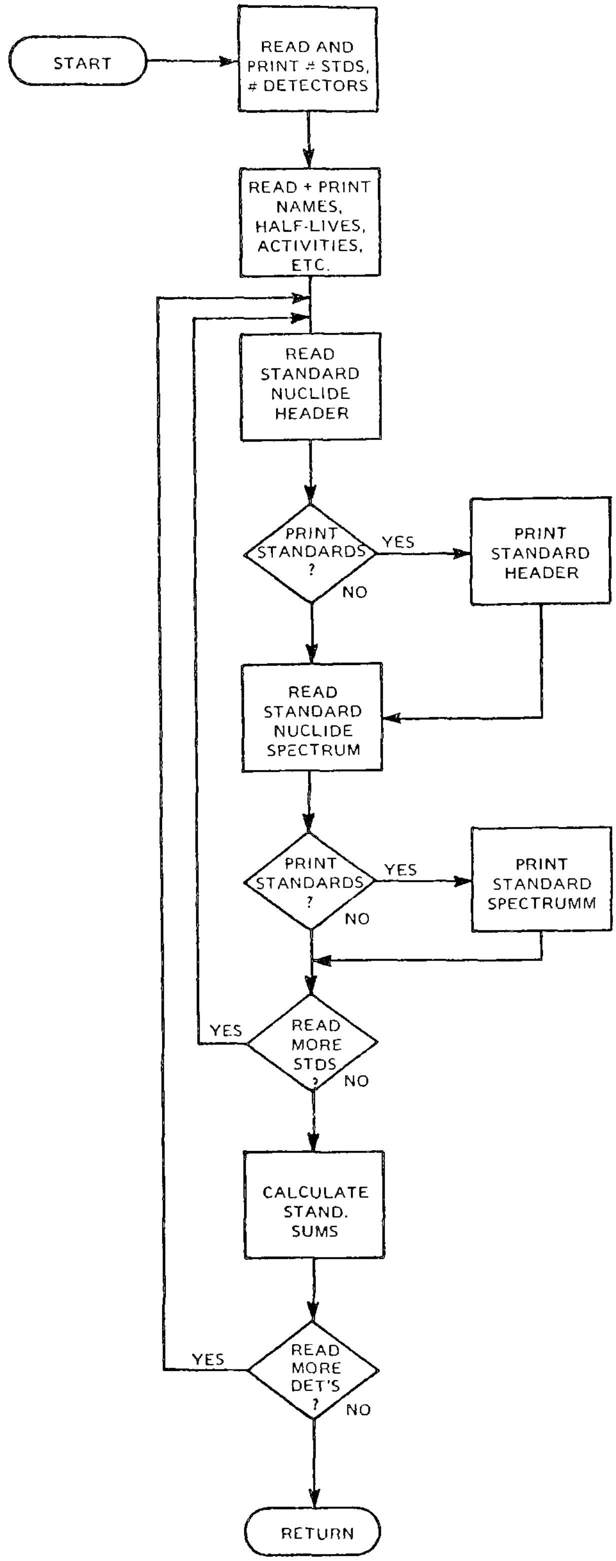

Figure A-3. ALPHA-M subroutine STDIN flow diagram.

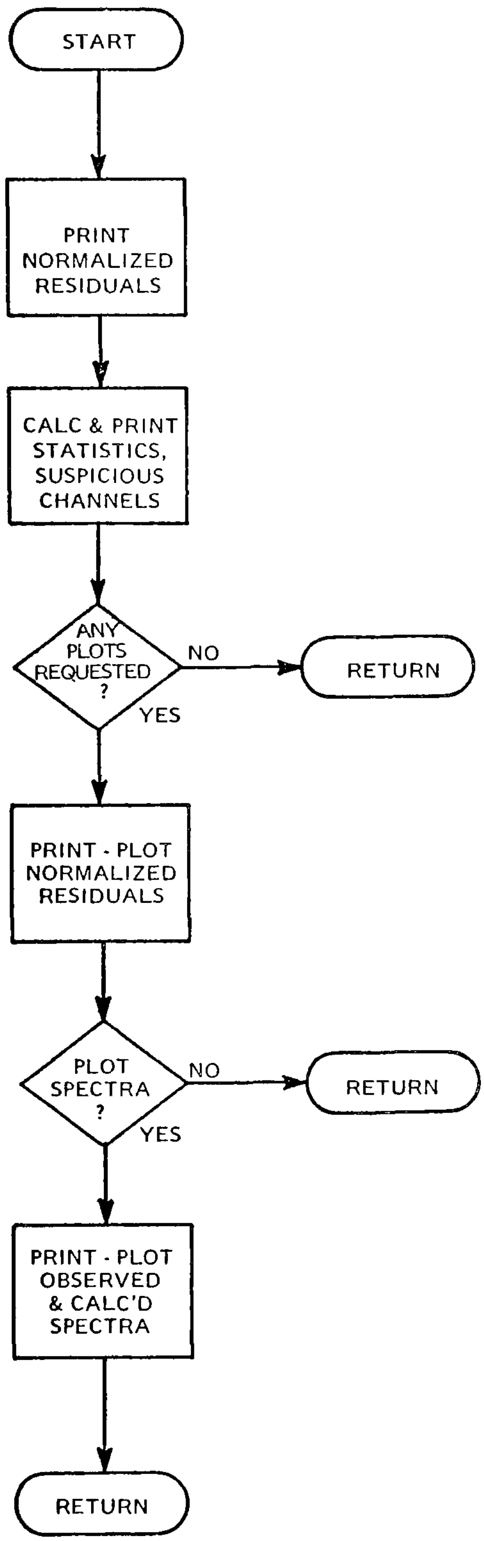

Figure A-4. ALPHA-M subroutine RESIDU flow diagram.

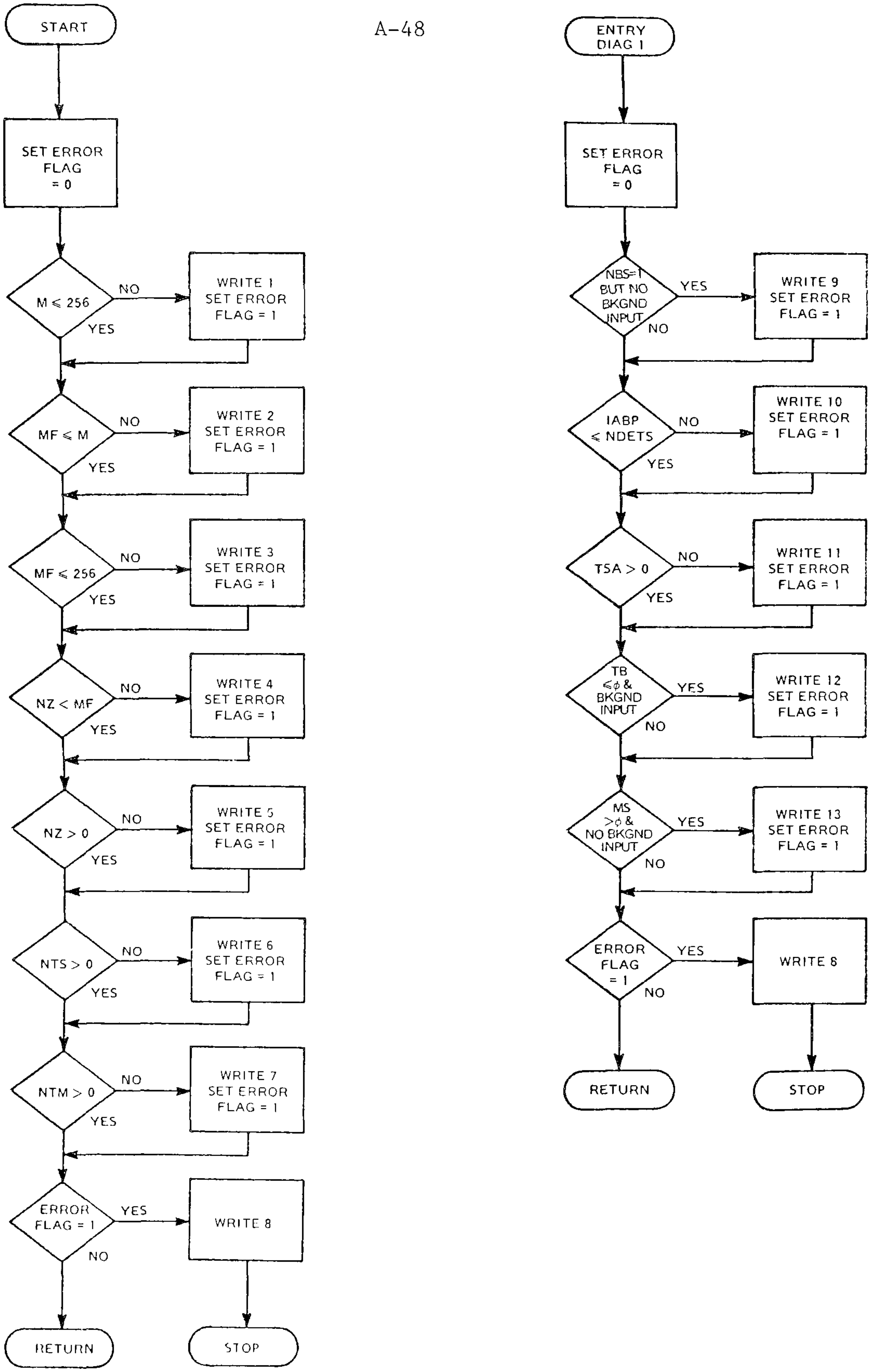

Figure A-5. ALPHA-M subroutine DIAG flow diagram.

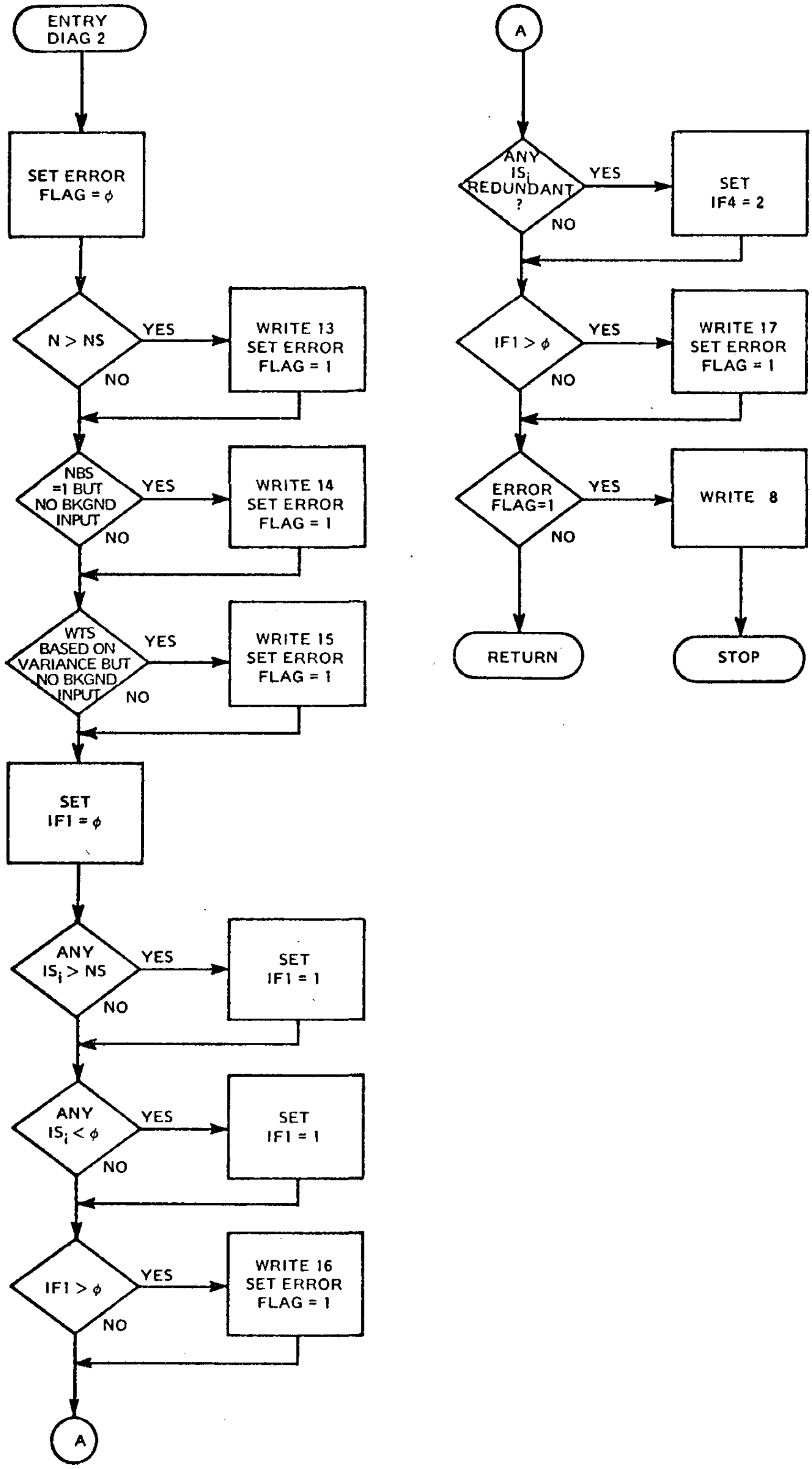

Figure A-5. ALPHA-M subroutine DIAG flow diagram (cont.)

APPENDIX B

GEN4

B.1 INTRODUCTION

Program GEN4 was written to provide a means of easily creating and updating the standard nuclide library. This reference library may be constructed to contain up to 20 standard spectra (of 256 channels each) for one to four detector geometries. A standard background spectrum may be created by submitting to GEN4 a number of background spectra that are then averaged. Reference spectra may be supplied to GEN4 with the sample background previously subtracted by the analyzer, or a standard background may be calculated by the program and subtracted from all input spectra. In addition, the library produced by GEN4 contains all data regarding names, half-lives, counting times, and activities of the standard nuclides.

Operating in the update mode, the program can replace any library standard spectrum and its identifying header. Since it is assumed that such changes will be made to the background only, there has been included no provision to modify the appropriate information record (activity, name, half-life, etc.) for the specified standard.

Printed output from GEN4 includes all information recorded on the information records as well as tabulated values for all standard spectra input. The sum of all channels in each spectrum is also displayed.

To increase the size of the standard nuclide library to more than 20 nuclides requires that the following variables be redimensioned: TST, TISOT, HA, and AC. For more than four detectors, the variables AC and NDN must be dimensioned accordingly. In addition, program lines 190-210 must have the value of K adjusted for the desired number of detectors. Additional lines of code must be added after line 110 to name the added detectors. Lines 80-110 name the first 4 detectors (detectors A, B, C, and D). The values 193, 194, 195, and 196 are the integer equivalents for the alphabetic characters A, B, C, and D on the IBM-370.

To vary the number of data channels in the standard spectra, variables SPECT, BKGND, and AVBK must be redimensioned. The DO LOOP indices on lines 270, 330, 370, 510, 560, 1200, 1270, 1300, and 1400 must be changed.

B.2 STANDARD NUCLIDE LIBRARY

The standard nuclide library is a file of unformatted variable-length blocked records containing the title of the library; the number of standards and detector sets it contains; the names, halflives, counting times, and activities of all standard nuclides; and a descriptive header and spectrum for all standard nuclides. The format and organization of this file are described in the following paragraphs.

B.2.1 Type 1 Record

The first record in the file contains the variables LIB, NS, and NDETS. LIB is an integer vector of dimension three and contains a 12-character description, or title, of the library. The variables NS and NDETS are 4-byte integer numbers containing, respectively, the number of standards in a detector-geometry set, and the number of such sets. This record is 20 bytes in length. Information on this record is read by ALPHA-M and is included in its printout to serve as verification that the user has accessed the proper standard nuclide library (there may be several).

B.2.2 Type 2 Record

This record contains information regarding all library standards and is written according to the form

(TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,NS)

TISOT is a singly dimensioned, double precision variable that contains the alphanumeric name of each standard nuclide. The singly dimensioned variables HA and TST contain the half-lives (in days) of all the nuclides and the standard counting times (in minutes), respectively. The array AC (dimensioned 20 x 4) contains the activities as counted by each detector. That is, variable AC(4,2) would contain the activity of standard nuclide number 4 when counted by detector number 2. If there were three standard nuclides for each detector set (i.e., NS=3), this second type of record would appear as

TISOT(1),HA(1),TST(1),AC(1,1),AC(1,2),AC(1,3),AC(1,4),
TISOT(2),HA(2),TST(2),AC(2,1),AC(2,2),AC(2,3),AC(2,4),
TISOT(3),HA(3),TST(3),AC(3,1),AC(3,2),AC(3,3),AC(3,4).

The information contained on this record is read by ALPHA-M and is necessary for the analysis of sample spectra. It is also on the ALPHA-M printout to provide library verification for the user. Where there are less than four detector sets, the unused locations will be padded with zeros. Under an arrangement of 14 standards, the record is 448 bytes long.

B.2.3 Type 3 Records

After the first two records, the identifying headers and the spectra for each of the standard nuclides for each detector-geometry set will follow. Each header record will consist of an 80-byte alphanumeric description of the nuclide spectrum immediately following it. The types of information usually contained on this header record include the name of the nuclide, its activity, the detector number, and the time and date on which the standard was counted. This information is for the benefit of the user; it is not read in detail by ALPHA-M or any other existing software. Each sample spectrum resides on a single 1024-byte record immediately following its respective header. All channel contents are written as 4-byte real numbers. The type 3 records are organized sequentially according to detector-geometry sets; that is, all headers and spectra for nuclides 1 through NS of detector set 1 are followed by all headers and spectra for nuclides 1 through NS of detector set 2, etc. The last nuclide spectrum in each detector set (that is, nuclide number NS) is assumed to be the standard averaged background prepared by GEN4. For a library containing three detector sets of four standard nuclides each, the library file would be organized as shown in table B-1.

The total length of the type 3 records will be NDETS*(NS*1104) bytes; therefore, with 14 standards and 2 detectors, the length would be 30,912 bytes.

The standard nuclide file should be created with a record format of VBS, a record length of 1028 bytes, and a blocksize of 2060 bytes. According to the functions specified in the program, this file may be used as output only or as input and output.

TABLE B-1. STRUCTURE OF STANDARD NUCLIDE FILE

Type 1 Record, Library definition information
Type 2 Record, Standard nuclide information
Header for Std. Nuclide 1, Detector 1
Spectrum for Std. Nuclide 1, Detector 1
Header for Std. Nuclide 2, Detector 1
Spectrum for Std. Nuclide 2, Detector 1
Header for Std. Nuclide 3, Detector 1
Spectrum for Std. Nuclide 3, Detector 1
Header for Std. Nuclide 4, Detector 1
Spectrum for Std. Nuclide 4, Detector 1
Header for Std. Nuclide 1, Detector 2
Spectrum for Std. Nuclide 1, Detector 2
Header for Std. Nuclide 2, Detector 2
Spectrum for Std. Nuclide 2, Detector 2
Header for Std. Nuclide 3, Detector 2
Spectrum for Std. Nuclide 3, Detector 2
Header for Std. Nuclide 4, Detector 2
Spectrum for Std. Nuclide 4, Detector 2
Header for Std. Nuclide 1, Detector 3
Spectrum for Std. Nuclide 1, Detector 3
Header for Std. Nuclide 2, Detector 3
Spectrum for Std. Nuclide 2, Detector 3
Header for Std. Nuclide 3, Detector 3
Spectrum for Std. Nuclide 3, Detector 3
Header for Std. Nuclide 4, Detector 3
Spectrum for Std. Nuclide 4, Detector 3

B.3 GEN4 INSTRUCTIONS

GEN4 input instructions are provided in table B-2; GEN4 update instructions are provided in table B-3.

TABLE B-2. GEN4 INPUT INSTRUCTIONS

(Library Information Card)

Variable	Columns	Format	Description
LIB	1-12	3A4	Twelve character identifier for library type. If the word "UPDATE" is punched in columns 1-6, however, the remainder of the card is ignored and all subsequent instructions come from those described in "Update Instructions."
NS	15-19	I5	Number of standard nuclides in a detector set.
NDETS	20-24	I5	Number of detector sets in library.
FMT	30-69	10A4	The format under which the standard spectra and backgrounds are to be read.

(Standards Information Cards, Set of NS Cards)

Variable	Columns	Format	Description
TISOT	1-8	A8	Name of standard nuclide
HA	9-18	F10.0	Half-life (days) of standard nuclide
TST	19-28	F10.0	Counting time (minutes) for nuclide
AC	29-38	F10.0	Activity (pCi/unit) for nuclide, detector 1
AC	39-48	F10.0	Activity (pCi/unit) for nuclide, detector 2
AC	49-58	F10.0	Activity (pCi/unit) for nuclide, detector 3

TABLE B-2 (cont.)

(Standards Information Cards, Cont.)

Variable	Columns	Format	Description
AC	59-68	F10.0	Activity (pCi/unit) for nuclide , detector 4

(Background Information Card)

Variable	Columns	Format	Description
NBKS	1-5	I5	Number of background spectra to read in and average.
NSUB	6-10	I5	0 = Do not subtract an average background spectrum from each standard nuclide spectrum as it is read in. 1 = Subtract an average background spectrum from all standards read in.

(Background Spectrum Cards)

NBKS sets of cards with each set consisting of the following:

1. Background header card - (20A4)
2. Background spectrum punched on as many cards as necessary according to the format specified on the library information card.

(Standard Spectra Cards)

NS-1 sets of cards with each set consisting of the following:

1. Standard header card - (20A4)
2. Standard spectrum(i) punched on as many cards as necessary according to the format specified on the library information card.

TABLE B-3. GEN4 UPDATE INSTRUCTIONS

(Update Control Card)

Variable	Columns	Format	Description
NDET	1-5	I5	Number of detector set to be updated.
NSTD	6-10	I5	Number of library standard to be replaced.
NBKS	11-15	I5	Number of background spectra to read in and average.

(Format Card)

Variable	Columns	Format	Description
FMT	1-40	10A4	Format under which the background spectra are to be read.

(Background Header Card)

Variable	Columns	Format	Description
NBHEAD	1-80	20A4	Header for new background spectrum std.

(Background Spectra Cards)

NBKS sets of cards with each set consisting of the following:

1. Background header card - (20A4)
2. Background spectrum, punched on as many cards as necessary, according to the format specified on the format card.

Note: For each detector background to be updated, a set of the above cards must be included.

B.4 GEN4 PROGRAM

The GEN4 program is provided in the following computer printout.

GEN4 PROGRAM

```
C*************************************************************************
C
C      GENERATES STANDARD NUCLIDE SPECTRUM LIBRARY
C
C*************************************************************************
      REAL*8 TISOT(20)
      DIMENSION HA(20),TST(20),AC(20,4),SPECT(256),BKGND(256),FMT(10),
     $NAME(20),NBHEAD(20),LIB(3),AVBK(256),NDN(4)
      COMMON/A/TISOT,HA,TST,AC,SPECT,BKGND,FMT,NAME,NBHEAD,LIB,AVBK
      DATA KEY/'UPDA'/
C
      WRITE(6,101)
      NDN(1) = 193
      NDN(2)   194
      NDN(3) - 195
      NDN(4) = 196
      READ(5,100) LIB,NS,NDETS,FMT
      IF (LIB(1).EQ.KEY) CALL UPDATE
      WRITE(6,102) LIB,NS,NDETS
      WRITE(9) LIB,NS,NDETS
C
      WRITE(6,105)
      DO 5 I=1,NS
      READ(5,104) TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4)
5     WRITE(6,106) TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4)
      WRITE(9)(TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,NS)
C
      DO 50 K=1,NDETS
      READ(5,108) NBKS,NSUB
      READ(5,110) NBHEAD
      WRITE(6,103) NDN(K),NBKS,NSUB,NBHEAD
      DO 8 I=1,256
8     AVBK(I)   0.0
      DO 10 J=1,NBKS
      READ(5,110)
      READ(5,FMT) BKGND
      WRITE(6,118) BKGND
      DO 10 I=1,256
10    AVBK(I) = AVBK(I) + BKGND(I)
      XNBKS   NBKS
      TSPEC = 0.0
      DO 20 I=1,256
      AVBK(I)   AVBK(I)/XNBKS
20    TSPEC   TSPEC + AVBK(I)
      WRITE(6,119) NDN(K),AVBK
      WRITE(6,117) TSPEC
C
C
      NSB = NS - 1
      DO 40 I=1,NSB
      READ(5,110) NAME
      READ(5,FMT) SPECT
      TSPEC = 0.0
      IF (NSUB.EQ.0) GO TO 32
C
      DO 31 J=1,256
      SPECT(J) - SPECT(J) - AVBK(J)
31    TSPEC   TSPEC + SPECT(J)
      GO TO 34
C
```

GEN4 PROGRAM (Cont.)

```
32    DO 33 J=1,256
      IF (SPECT(J).GT.900000.) SPECT(J)   SPECT(J) - 1000000.
33    TSPEC   TSPEC + SPECT(J)
C
34    WRITE(6,112) NAME,NDN(K)
      WRITE(6,116) SPECT
      WRITE(6,117) TSPEC
      WRITE(9) NAME
40    WRITE(9) SPECT
      WRITE(9) NBHEAD
      WRITE(9) AVBK
C
50    CONTINUE
C
100   FORMAT(3A4,T15,2I5,T30,10A4)
101   FORMAT('1GEN4 - - STANDARD SPECTRUM LIBRARY GENERATION - - RADIOAN
     $ALYTICAL LABORATORY',///)
102   FORMAT('0',' GEOMETRY LIBRARY TYPE - ',3A4,10X,
     $ 'NUMBER OF LIBRARY STDS IS ',I2,10X,
     $'NUMBER OF DETECTORS IS ',I2)
103   FORMAT('1FOR DETECTOR',A4,'  NUMBER OF BKGND SPECTRA TO BE AVERAGE
     $D IS',I3,'   BKGND SUBTRACTION FLAG IS',I2,//,
     $' HEADER TO FILE IS  ',20A4)
104   FORMAT(A8,6F10.2)
105   FORMAT(/,1X,'NUCLIDE',4X,'HALF-LIFE(DAYS)',3X,
     $'CNT-TIME(MINS)',4X,'ACT-DET-A',4X,'ACT-DET-B',4X,
     $'ACT-DET-C',4X,'ACT-DET-D',/)
106   FORMAT(1X,A8,5X,F10.1,7X,F10.5,6X,F10.1,3X,F10.1,3X,F10.1,3X,F10.1
     $)
108   FORMAT(2I5)
110   FORMAT(20A4)
112   FORMAT('1',1X,20A4,T100,'DETECTOR',A4,/)
114   FORMAT(10F7.0)
116   FORMAT(1X,10F12.1)
117   FORMAT('0SUM OF CHANNELS IS ',F9.1)
118   FORMAT(/,/,/,(1X,10F12.1))
119   FORMAT(1H1,' AVERAGE BACKGROUND FOR DETECTOR',A4,
     $/,/,(1X,10F12.1))
C
      STOP
      END
      SUBROUTINE UPDATE
C
      REAL*8 TISOT(20)
      DIMENSION HA(20),TST(20),AC(20,4),SPECT(256),BKGND(256),FMT(10),
     $NAME(20),NBHEAD(20),LIB(3),AVBK(256),NDN(3)
      COMMON/A/TISOT,HA,TST,AC,SPECT,BKGND,FMT,NAME,NBHEAD,LIB,AVBK
      DIMENSION NHEAD(20,20,4), SPCTRA(256,20,4)
C
      WRITE(6,150)
      READ(9) LIB,NS,NDETS
      READ(9) (TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,NS)
C
      DO 10 I=1,NDETS
      DO 10 J=1,NS
      READ(9) (NHEAD(K,J,I),K=1,20)
10    READ(9) (SPCTRA(K,J,I),K=1,256)
C
      REWIND 9
      WRITE(9) LIB,NS,NDETS
```

GEN4 PROGRAM (Cont.)

```
      WRITE(9) (TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,NS)
C
20    READ(5,100,END=35) NDET,NSTD,NBKS,FMT,NBHEAD
      WRITE(6,151) NDN(NDET),NSTD,NBKS,FMT,NBHEAD
      DO 22 I=1,256
22    AVBK(I)  0.0
C
      DO 25 I=1,NBKS
      READ(5,152) NAME
      READ(5,FMT) BKGND
      WRITE(6,101) BKGND
      DO 25 J=1,256
25    AVBK(J)   AVBK(J) + BKGND(J)
      XNBKS   NBKS
      DO 30 I=1,256
      AVBK(I)   AVBK(I)/XNBKS
30    SPCTRA(K,NSTD,NDET)   AVBK(I)
      WRITE(6,102) NDN(NDET),NSTD,AVBK
C
      GO TO 20
C
35    DO 40 I=1,NDETS
      DO 40 J=1,NS
      WRITE(9) (NHEAD(K,J,I),K=1,20)
40    WRITE(9) (SPCTRA(K,J,I),K=1,256)
C
100   FORMAT(3I5,10A4,/,20A4)
101   FORMAT(/,/,/,(1X,10F12.1))
102   FORMAT('1FOR DETECTOR',A4,' - STANDARD NUMBER',I3,'  - THE AVERAGE
     $IS AS FOLLOWS:',/,(1X,10F12.1))
150   FORMAT (/,' THIS IS A BACKGROUND UPDATE RUN')
151   FORMAT(//,' FOR DETECTOR',A4,' - REPLACEMENT OF STD NUMBER',I3,' W
     $ILL BE BY AVERAGE OF ',I3,' SPECTRA',/,
     $' WHICH ARE INPUT WITH A FORMAT OF ',10A4,/,
     $' HEADER: ',20A4)
152   FORMAT (20A4)
      STOP
      END
```

B.5 GEN4 FLOW DIAGRAM

The GEN4 flow diagram is provided as figure B-1.

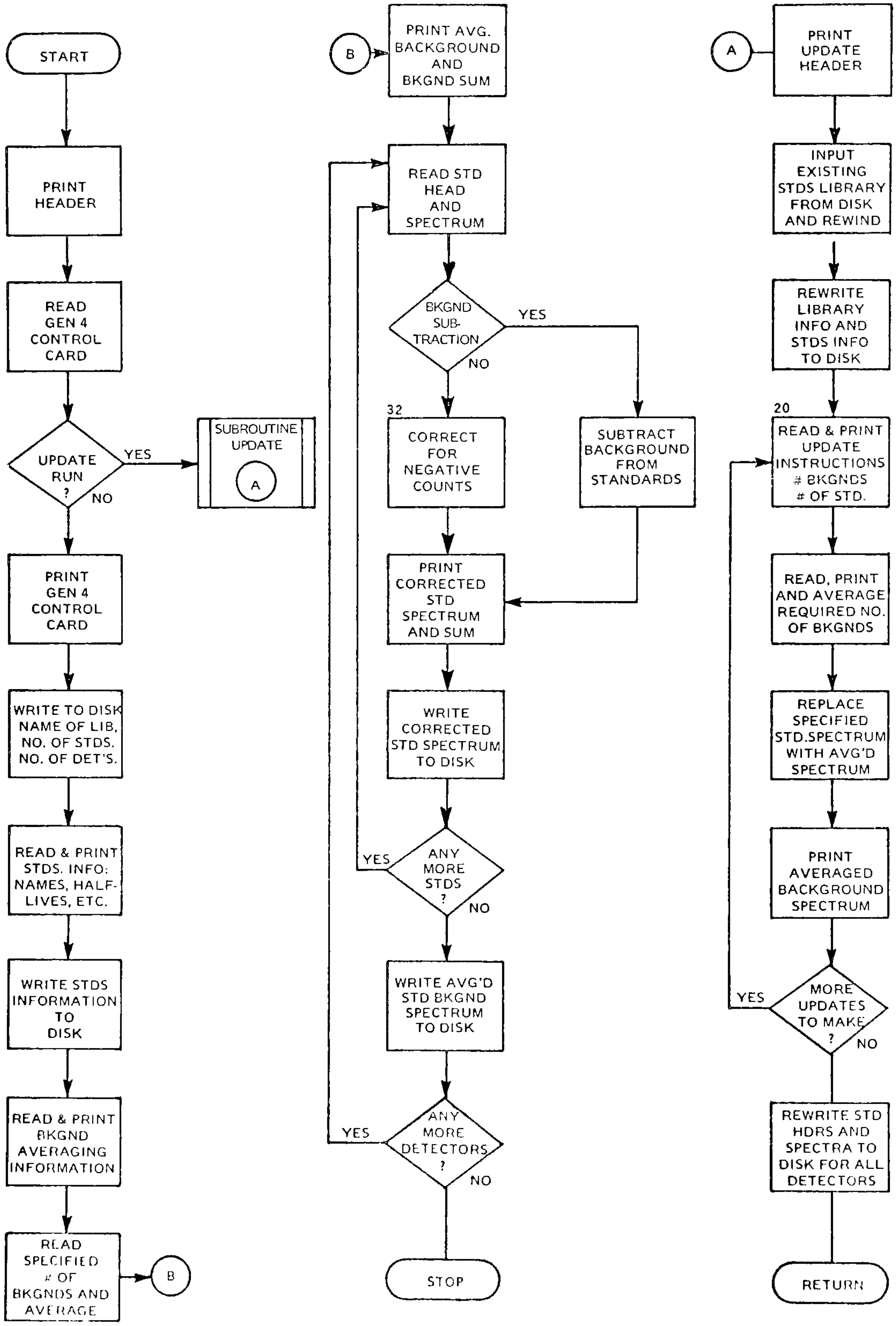

Figure B-1. GEN4 flow diagram.

APPENDIX C

SIMSPEC

C.1 INTRODUCTION

The program SIMSPEC was written to simulate mathematically sample spectra for ALPHA-M analysis. Operating on the information contained in the standard nuclide library, the program can generate multinuclide spectra with components at any specified activity level. The pure composite spectrum thus obtained may be operated on by channel randomization to simulate the effects resulting from normal counting statistics, and by specified degrees of gain and energy threshold shifting. Input instructions are included.

Each component is generated with a specified nuclide at the desired activity level by multiplying its standard spectrum by the ratio of the input (desired) activity to the level of that standard in the library. Composites are obtained by combining all required components in an additive manner. If so directed by program input, the spectrum is then randomized.

Assuming the availability of a pseudorandom number generator producing numbers x_i in the range 0 to 1.0, an approximation to normally distributed random numbers J_i may be generated with the expression

$$J_i = \frac{\sum^{N} \left(x_i - \frac{N}{2} \right)}{\left[N/12 \right]^{\frac{1}{2}}} * S + M \quad , \qquad (C1)$$

where S and M are the standard deviation and mean of the desired population, respectively, and N specifies the number of summations. Applying this operation to the randomization of the counts in each spectrum channel, we have

$$Y_{new} = \frac{\sum \left(x_i - \frac{N}{2} \right)}{\left[N/12 \right]^{\frac{1}{2}}} *SIGW* \left(Y_{old} \right)^{\frac{1}{2}} + Y_{old} \quad , \qquad (C2)$$

where Y_{old} and Y_{new} are the contents of a specified channel before and after randomization. The quantity $(Y_{old})^{\frac{1}{2}}$ will be recognized as the estimate of a one standard deviation error as produced by Poisson counting statistics. The use of the SIGW value, which controls the randomization process, is explained in the SIMSPEC input instructions.

The pseudorandom number generator used to produce the values x_i is the subroutine RANDU, written in Fortran and supplied in the IBM Scientific Subroutine Package, Version 3. This subroutine uses the congruence technique for random number generation. For more information on generation and testing, see Abramowitz and Stegun, Handbook of Mathematical Functions, U.S. Department of Commerce, National Bureau of Standards, Applied Mathematics Series 55, 1968, R. W. Hamming, Numerical Methods for Scientists and Engineers, McGraw-Hill, New York, 1962; or Random Number Generation and Testing, IBM manual C20-3011.

The desired gain and threshold shifts are produced in the output spectrum by using Schonfeld's subroutine SHIFT. The gain of the spectrum may be altered by input variable F, the ratio of the measured gain divided by the desired gain. Threshold shifts are normally affected by the input variable SHC, which is the number of channels (or usually, fractions of a channel) by which the spectrum must be shifted. The energy threshold of the reference spectrum is expressed in input variable SH. This variable may be used to match a desired calibration between the reference and sample spectra. As shown in an earlier section of this report, no exact determination of the energy threshold shift may be made easily; hence, this SH value should be set equal to 0.0 except for experimental purposes. A more detailed discussion of the uses of these input variables may be found in SHIFT-M, A Computer Program for Shifting Gamma-Ray Spectra in Gain and Threshold by Linear Interpolation, an addition and revision to ORNL-3975, E. Schonfeld, 1966.

If randomization is requested, SIMSPEC will produce descriptive statistics of the body of random variates used to randomize the composite spectrum. These statistical tests are useful only for evaluating the randomizing process. In addition, the unrandomized spectra, randomized spectra, and the random variates may be, upon request, passed to an intermediate dataset for subsequent data processing. The program ANALYZE was used for this purpose, but is not included in this report. It is available from the authors as an object deck for the IBM Systems 360-370. ANALYZE is a nonstandard program that might not run in installations having other than IBM equipment.

C.2 SIMSPEC FILE UTILIZATION

C.2.1 Standard Nuclide Library

An input file always required. Refer to documentation regarding program GEN4.

C.2.2 Auxiliary Output File

An output file is required if SIMSPEC input variable IRX is greater than zero and if randomization is requested (SIGW ≠ 0). If this option is selected, a binary unformatted record is written on Fortran logical unit IRX at the end of each sample spectrum generation cycle. The record contains the variables XIDT, R, YC, and SPEC, where XIDT is the sample identification (8 bytes, alphanumeric), and R, YC, and SPEC are vectors (each output as 256 locations) containing, respectively, the vector of random variates, the shifted randomized spectrum, and the original composite generated by SIMSPEC. The file consisting of these records is equivalent to its counterpart in program ALPHA-M, and the same DCB and storage considerations apply.

C.2.3 Primary Output File

A required file containing all SIMSPEC generation output and intended for input to program ALPHA-M, the file consists of variable-length, blocked records formatted as card images and described with a DCB=(RECFM=FB,LRECL=80,BLKSIZE=800). With this structure, approximately 140 records may be written onto each 3330-type track. An ALPHA-M run containing 10 samples with one analysis option each, assuming 26 card images for each sample and the background spectrum, will require 319 records.

C.3 JOB CONTROL LANGUAGE REQUIREMENTS

In the course of this study, an instream Job Control Language procedure (called SIMALPH) was used to allocate required datasets and execute the programs in the proper order. A general description of these procedures should serve to illustrate the requirements of the software used. It is assumed that the reader is familiar with the usage and syntax of IBM OS Job Control Language.

SIMALPH consists of four steps (figure C-1). The first, SIM, executes the program SIMSPEC. SIMSPEC receives its input instructions from the card reader (FTØ5FØØ1), uses information contained in the standard nuclide library (FTØ2FØØ1), and writes input instructions and generated samples onto a temporary dataset (FTØ3FØØ1, DSN=XFER) for ALPHA-M to receive. Simultaneously, SIMSPEC creates another temporary dataset (FTØ4FØØ1, DSN=RESID) containing the residuals between the pure and randomized spectra generated, for processing by program ANALYZE.

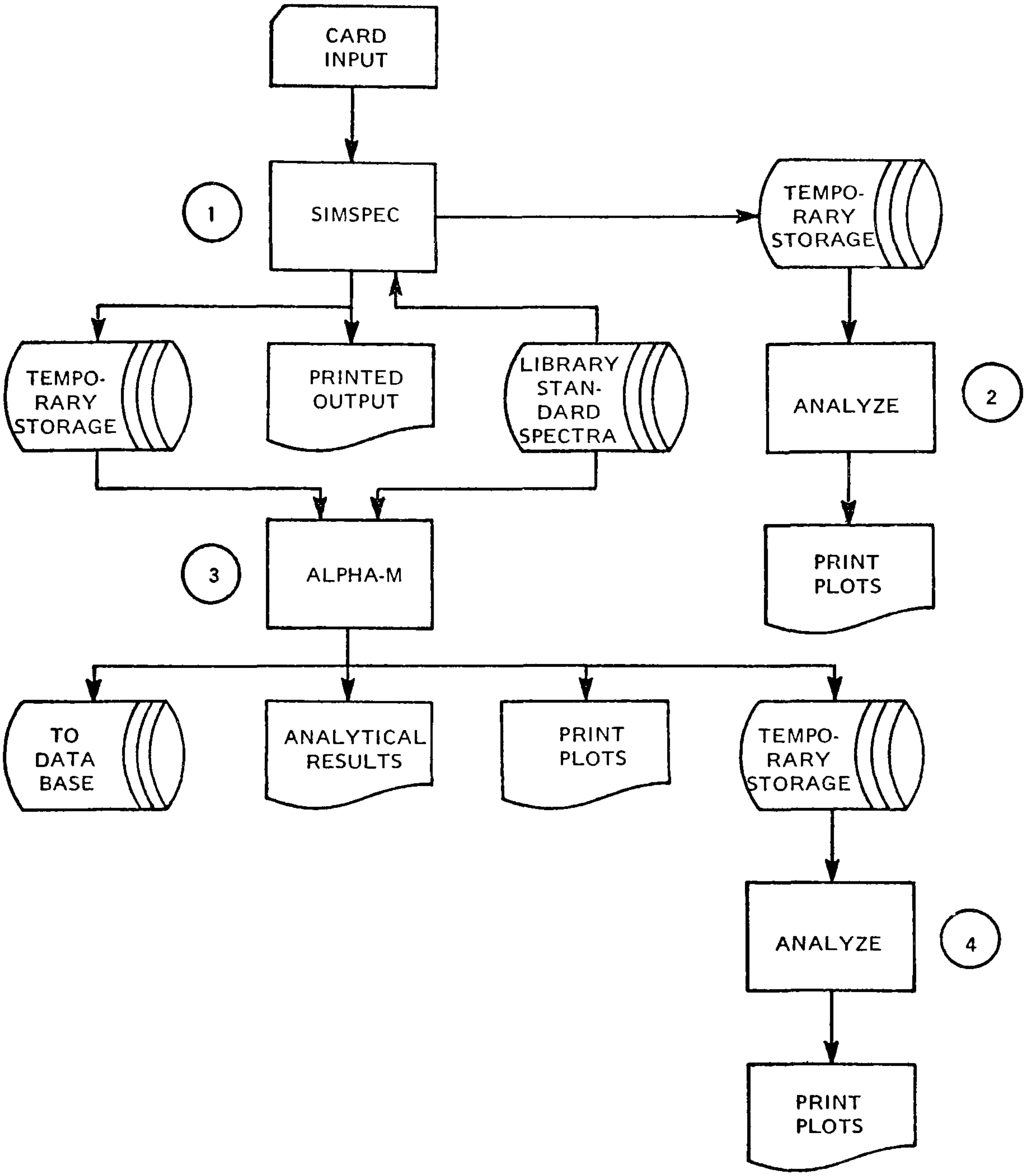

Figure C-1. Program-file dependency in SIMALPH.

In step two, ANALYZE is executed to evaluate the residuals passed to it, and, when finished, to delete this temporary dataset. The program's output consists of print-plots that are produced on a printer dataset.

ALPHA-M is executed in step three. The program receives input instructions and samples via dataset XFER (FT05F001) that is then deleted, uses information contained in the standards library (FT03F001), produces analytical results on one printer dataset (FT06F001), print-plots on another (FT09F001), creates temporary storage for residuals (FT04F001), and outputs analytical data (FT02F001) for entry into a data base. In this step, Fortran logical unit 2 (analytical results to data base) is defined as a temporary dataset. For a production application, this disposition would be defined as (MOD,KEEP) for continuous addition of data.

In step four, the program ANALYZE is again executed to evaluate the residuals produced by ALPHA-M. The output from ANALYZE is again produced on a printer dataset and, at termination, the temporary storage (FT02F001, DSN=RESID) passed from step 3 (ALPHA) is deleted.

The DDnames used in this procedure are contingent upon the following input instructions being supplied to the programs involved. For SIMSPEC, IRX must be set equal to 4. For ALPHA-M, NTS=3, NTM=5, IAUX=4, and IOPT=2. The use and application of Fortran logical units 2 and 3 in SIMSPEC, unit 9 in ALPHA-M, and unit 2 in ANALYZE, are internally fixed. The standard definitions of units 5 and 6 for card reader and line printer are employed in all programs.

C.4 SIMSPEC INPUT INSTRUCTIONS

SIMSPEC input instructions are provided in table C-1.

TABLE C-1. SIMSPEC INPUT INSTRUCTIONS

(General Control Cards - 3I10)

Variable	Columns	Format	Description
IX	1-10	I10	Seed integer for randomization, must be one to nine digits, odd.
IRX	11-20	I10	If IRX greater than zero, residuals will be output on Fortran logical unit IRX.
IRANGE	21-30	I10	Number of terms over which randomization will be summed, see text.
IWRITE	31-40	I10	0 = For no print-plot of spectra 1 = To print-plot spectra

(ALPHA-M General Control Card)

Refer to table 1.

(ALPHA-M Sample Control Card)

Refer to table 1.

TABLE C-1 (cont.)

(Background Information Cards)

Only if ALPHA-M variable NBR is greater than zero.

1. Background title card, format (20A4)
2. Background component card, format (I2,7X,I1,T15, F10.0) with the following information:

Variable	Columns	Format	Description
NBK	1-2	I2	The library number of the library standard spectrum to use for the background.
NDT	10	I1	The number of the detector set in which the desired spectrum resides.
XPCI	15-24	F10.0	The number of pCi/unit activity desired for the background.

(Sample Information Cards)

1. Sample title card, format (20A4)
2. Sample component cards, format (I2,(T9,I2,T20,I1,T30, F10.0)) with the following information:

Variable	Columns	Format	Description
NO	1-2	I2	The number of components which are to comprise the generated spectrum. This variable appears only on the first of the NO sample component cards, the subsequent NO-1 cards should contain blanks in columns 1-2.
NSTD	9-10	I2	The number of the library standard to be used for component i.
NDET	20	I1	The number of the detector set in which the desired standard resides.
PCI	30-39	F10.0	The desired activity level for component i.

TABLE C-1 (cont.)

(Shifting and Randomization Control Card, Format (4F10.0)

Variable	Columns	Format	Description
F	1-10	F10.0	Gain factor (gain actual/gain desired)
SH	11-20	F10.0	Reference threshold channel (normally zero; used if it is desired to adjust the spectrum to a specific calibration).
SHC	21-30	F10.0	Energy threshold shift to apply; number of channels or fractions of a channel by which the spectrum will be shifted.
SIGW	31-40	F10.0	0 = For no randomization 1.0 = For randomization as illustrated in the text; intermediate values will have the effect of changing the magnitude of the std. dev. of the distribution.

(ALPHA-M Option Card)

Same as in ALPHA-M (refer to table 1) as many cards specified by NOPT on ALPHA-M sample control card.

C.5 SIMSPEC PROGRAM

The SIMSPEC program is provided in the following computer printout.

SIMSPEC PROGRAM

```
C*************************************************************************
C
C        ...SIMSPEC...
C        PROGRAM TO SIMULATE COMPOSITE, RANDOMIZED, SHIFTED GAMMA-RAY
C        SPECTRA AND PREPARE INPUT FOR PROGRAM ALPHA-M.
C        TENNESSEE VALLEY AUTHORITY, RADIOLOGICAL HYGIENE BRANCH, 1976
C
C*************************************************************************
      INTEGER FM,TNAME
      REAL*8 XIDT,TISOT
      DIMENSION L1(3),TISOT(22),HA(22),TST(22),AC(22,4),IS(22),PCI(22),
     $TNAME(20),S(20,256,4),FM(8),SPECT(267),PCT(22),NSTD(22),NDET(22),
     $YC(257),BK(257),XFRQ(20),R(256),SPEC(257),X(20),PROB(20),
     $GFREQ(20)
      DATA SPECT/267*0.0/,J/0/
C
C     READ INPUT INSTRUCTIONS
C
      READ(5,300) IX,IRX,IRANGE,IWRITE
      WRITE(6,310) IX,IRX,IRANGE,IWRITE
      XFACT   IRANGE/2.0
      DIV = SQRT(FLOAT(IRANGE)/12.0)
C
C     READ DISK DETECTOR STANDARDS LIBRARY INFORMATION
C
      READ(2) L1,L2,L3
      WRITE(6,100) L1,L2,L3
      READ(2) (TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,L2)
      WRITE(6,110)
      WRITE(6,120) (TISOT(I),HA(I),TST(I),(AC(I,K),K=1,4),I=1,L2)
      DO 10 K=1,L3
      DO 10 I=1,L2
      READ(2) TNAME
10    READ(2) (S(I,J,K),J=1,256)
      NS   L2
      NDETS   L3
C
C     READ GENERAL CONTROL CARD
C
      READ(5,130) M,NIT,NBA,NZ,MF,NTS,NTM,MU,NH,IAUX,IOPT,FM
      WRITE(6,140)M,NIT,NBA,NZ,MF,NTS,NTM,MU,NH,IAUX,IOPT,FM
      WRITE(3,130)M,NIT,NBA,NZ,MF,NTS,NTM,MU,NH,IAUX,IOPT,FM
C
      DO 50 K=1,50
C
C     READ SAMPLE CONTROL CARD
C
      READ(5,150,END=900) XIDT,NOPT,NBR,NBS,IABP,MS,TB,TSA,VRED,DAY,VM
      WRITE(6,160) K,XIDT,NOPT,NBR,NBS,IABP,MS,TB,TSA,VRED,DAY,VM
      WRITE(3,150) XIDT,NOPT,NBR,NBS,IABP,MS,TB,TSA,VRED,DAY,VM
      IF (NBR) 30,30,20
C
C     IF SPECIFIED, READ BACKGROUND HEADER AND COMPONENT
C
20    READ(5,170) TNAME
      WRITE(6,180) TNAME
      WRITE(3,170) TNAME
      READ(5,190) NBK,NDT,XPCI
      XPCT   XPCI/(AC(NBK,NDT)/VRED)
      WRITE(6,210) XPCI,NBK,NDT
```

SIMSPEC PROGRAM (Cont.)

```
      DO 25 J=1,256
25    BK(J)    S(NBK,J,NDT)*XPCT
      WRITE(6,200) (BK(N),N=1,256)
      WRITE(3,FM) (BK(N),N=1,256)
      WRITE(6,220)
C
C     READ SAMPLE HEADER, COMPONENTS, AND SHIFTING INFORMATION
C
30    READ(5,170) TNAME
      WRITE(3,170) TNAME
      WRITE(6,180) TNAME
      READ(5,230) NO,(NSTD(I),NDET(I),PCI(I),I=1,NO)
      DO 34 I=1,NO
34    PCT(I)    PCI(I)/(AC(NSTD(I),NDET(I))/VRED)
      WRITE(6,240) (PCI(I),NSTD(I),NDET(I),I=1,NO)
      READ(5,270) F,SH,SHC,SIGW
      WRITE(6,280) F,SH,SHC,SIGW
      DO 35 J=1,256
35    SPECT(J)    0.0
C
C     COMPUTE COMPOSITE SAMPLE SPECTRUM
C
      DO 40 J=1,256
      DO 40 I=1,NO
40    SPECT(J) = SPECT(J) + S(NSTD(I),J,NDET(I))*PCT(I)
      DO 141 J=1,256
141   SPEC(J) = SPECT(J)
C
C     OBTAIN VECTOR OF VARIATES AND RANDOMIZE SPECTRUM IN SPECT
C
      DO 42 I=1,256
      A = 0.0
      DO 41 J=1,IRANGE
      CALL RANDU (IX,IY,YFL)
      IX    IY
41    A    A + YFL
      R(I)    (A-XFACT)/DIV
42    SPECT(I)    R(I) * SQRT(ABS(SPECT(I))) * SIGW + SPECT(I)
C
C     APPLY SPECIFIED GAIN AND THRESHOLD SHIFTS AND RETURN IN VECTOR YC
C
      CALL SHIFT(SPECT,YC,F,SH,SHC,MX)
      IF (MX.GE.256) GO TO 44
      DO 43 I=MX,256
43    YC(I)    0.0
C
44    WRITE(6,200) (YC(N),N=1,256)
      WRITE(3,FM) (YC(N),N=1,256)
C
C     READ AND WRITE SPECIFIED NUMBER OF OPTION CARDS
C
      DO 45 J=1,NOPT
      READ(5,250) N,NB,NW,KT,IRD,IPRINT,CH,Q,XMOD,(IS(I),I=1,N)
      WRITE(3,250) N,NB,NW,KT,IRD,IPRINT,CH,Q,XMOD,(IS(I),I=1,N)
45    WRITE(6,260) N,NB,NW,KT,IRD,IPRINT,CH,Q,XMOD,(IS(I),I=1,N)
C
C     IF REQUESTED, PLOT PURE AND RANDOMIZED SPECTRA
C
      IF (IWRITE.EQ.0) GO TO 144
      CALL PLOT(K,SPEC,YC)
```

SIMSPEC PROGRAM (Cont.)

```
C
144   XRSUM = 0.0
      XSQSUM = 0.0
      SUMI   0.
      SUMT = 0.
      SIG1 = 0.
      SIG2 = 0.
      SIG3 = 0.
C
C     DESCRIPTIVE STATISTICS OF THE BODY OF VARIATES
C
      IF (SIGW) 145,50,145
145   DO 46 I=1,256
      XRSUM - XRSUM + R(I)
46    XSQSUM   XSQSUM + R(I)*R(I)
      XCBSUM   XCBSUM + R(I)*R(I)*R(I)
      X4TH - X4TH + R(I)*R(I)*R(I)*R(I)
      XNO = 256.
      RAVG   XRSUM/XNO
      RSIG=SQRT((1./(XNO-1.))*(XSQSUM-((XRSUM**2)/XNO)))
      DO 48 I=1,256
      SUMI   SUMI + ((R(I)-RAVG)/RSIG)**3
48    SUMT   SUMT + ((R(I)-RAVG)/RSIG)**4
      RSKEW = SUMI/XNO
      RKURT   SUMT/XNO
      DO 47 I = 1,256
      IF((R(I).LE.(3.*RSIG)).AND.(R(I).GE.(-3.*RSIG))) SIG3   SIG3 +1
      IF((R(I).LE.(2.*RSIG)).AND.(R(I).GE.(-2.*RSIG))) SIG2   SIG2 +1
47    IF((R(I).LE.(1.*RSIG)).AND.(R(I).GE.(-1.*RSIG))) SIG1   SIG1 +1
      SIG3 - (SIG3/256.)*100.
      SIG2   (SIG2/256.)*100.
      SIG1   (SIG1/256.)*100.
C
      WRITE(6,90) RAVG,RSIG,RSKEW,RKURT,SIG1,SIG2,SIG3
C
      IF(IRX.GT.0)WRITE(IRX)XIDT,J,R,(YC(I),I=1,256),(SPEC(I),I=1,256)
C
50    CONTINUE
C
C     FORMAT STATEMENTS
C*****************************************************************
C
90    FORMAT(/,' STATISTICS FOR VARIATES',/,
     $' AVERAGE =',F7.4,5X,'STD. DEV. =',F7.4,5X,'SKEWNESS =',F7.4,
     $5X,'KURTOSIS =',F9.4,/,' PERCENTAGE WITHIN 1 SIGMA =',F6.2,
     $5X,'2 SIGMA =',F6.2,5X,'3 SIGMA =',F6.2)
100   FORMAT(//,' INSTRUCTED TO USE FILE FOR GEOMETRY TYPE ',3A4,
     $10X,'CONTAINING ',I2,' STANDARDS FOR ',I1,' DETECTORS')
110   FORMAT(/,1X,'NUCLIDE',4X,'HALF-LIFE(DAYS)',3X,'CNT-TIME(MINS)',
     $3X,'ACT-DET-A',4X,'ACT-DET-B',4X,'ACT-DET-C',4X,'ACT-DET-D',/)
120   FORMAT(1X,A8,5X,F10.1,7X,F10.5,6X,F10.1,3X,F10.1,3X,F10.1,
     $3X,F10.1)
130   FORMAT(11I4,8A4)
140   FORMAT(/,' GENERAL CONTROL CARD',/,11I5,2X,8A4)
150   FORMAT(A8,5I3,5F9.4)
160   FORMAT(1H1,'SAMPLE NUMBER ',I2,/,' SAMPLE CONTROL CARD',
     $/,1X,A8,5I3,5F9.4,/)
170   FORMAT(20A4)
180   FORMAT(1X,20A4,/)
190   FORMAT(I2,7X,I1,T15,F10.0)
```

SIMSPEC PROGRAM (Cont.)

```
200   FORMAT(1X,10F12.1)
210   FORMAT(' BACKGROUND ',F8.1,' PCI/UNIT OF STANDARD',I3,' FOR DETECT
     $OR',I2,/)
220   FORMAT(1H1)
230   FORMAT(I2,(T9,I2,T20,I1,T30,F10.0))
240   FORMAT(' SAMPLE WILL CONSIST OF:',/,(1X,F8.1,' PCI/UNIT OF STANDAR
     $D',I3,' FOR DETECTOR',I2))
250   FORMAT(6I3,3F6.2,(22I2))
260   FORMAT(/,' OPTION CARD   ',6I4,3F6.2,(22I3))
270   FORMAT(4F10.0)
280   FORMAT(/,' GAIN SHIFT RATIO IS',F7.4,'   THRESHOLD CHANNEL IS ',
     $F4.0,'     THRESHOLD SHIFT IS ',F7.4,'     RAND FLAG IS ',F3.1)
300   FORMAT(8I10)
310   FORMAT(1X,131('*'),/,
     $40X,'SIMSPEC - DATA GENERATION - RADIOANALYTICAL LABORATORY',/.
     $1X,131('*'),/,
     $' SEED FOR RANDOM NUMBER GENERATOR IS',I10,
     $5X,'RESIDUAL OUTPUT FLAG IS',I3,5X,
     $'RANGE FOR SERIES IS',I4,'   IWRITE= ',I2)
900   STOP
      END
      SUBROUTINE SHIFT (Y,YC,F,SH,SHC,MX)
C
C     E. SCHOENFIELD, 1966
C
      DIMENSION Y(267),YC(257)
      TE    SH * (F-1.0)
      JT    1
      MX    F * (256+SHC) + TE + 1
3     DO 60 I=1,256
      QI    I
      DO 40 J=JT ,256
      Z = J
      QJ    F * (Z+SHC) + TE
      IF (QI-QJ) 41,45,40
41    IF (J-1) 45,45,50
45    YC(I)    Y(J)
      YT    J
      GO TO 60
40    CONTINUE
      GO TO 60
50    YC(I)    (Y(J)-Y(J-1))/F
      YC(I)    Y(J-1) + YC(I) * (QI-QJ+F)
      YC(I)    YC(I)/F
      JT = J
60    CONTINUE
      YC(1)    1.0
      WRITE(6,100) MX
100   FORMAT(' DATA MEANINGLESS AFTER CHANNEL',I4)
      RETURN
      END
      SUBROUTINE PLOT(K,A,B)
C
C     PLOT OF TWO FUNCTIONS, A   CALC'D, B   OBS'D, K   SAMPLE NO.
C
      DIMENSION A(257),B(257),LINE(101)
      INTEGER NBLNK/' '/,NPLUS/'+'/,NSTAR/'*'/
      WRITE(6,99) K
99    FORMAT(1H1,30X,'PLOT OF PURE COMPOSITE, AND SHIFTED/RANDOMIZED SPE
     $CTRA, SAMPLE NUMBER',I3,//,' CH  BEFORE   AFTER')
```

SIMSPEC PROGRAM (Cont.)

```
      XMAX   -1.0E20
      XMIN = 1.0E20
      DO 10 I=10,200
      IF (A(I).GT.XMAX) XMAX - A(I)
      IF (B(I).GT.XMAX) XMAX = B(I)
      IF (A(I).LT.XMIN) XMIN = A(I)
10    IF (B(I).LT.XMIN) XMIN - B(I)
      RANGE   XMAX-XMIN
      XINC = RANGE /100.
      DO 20 I=10,200
      DO 15 J   1,101
15    LINE(J)   NBLNK
      NPOS   (A(I)-XMIN)/XINC + 1
      LINE(NPOS) = NPLUS
      NPOS   (B(I)-XMIN)/XINC + 1
      LINE(NPOS) = NSTAR
20    WRITE(6,100) I,A(I),B(I),NSTAR,LINE,NSTAR
100   FORMAT(I4,2F8.1,103A1)
      RETURN
      END
      SUBROUTINE RANDU(IX,IY,YFL)
C     FROM SSP/360 V.3
      IY   IX * 65539
      IF (IY) 5,6,6
5     IY   IY + 2147433647 + 1
6     YFL   IY
      YFL = YFL * .4656613E-9
      RETURN
      END
```

C.6 SIMSPEC FLOW DIAGRAM

The SIMSPEC flow diagram is provided as figure C-2.

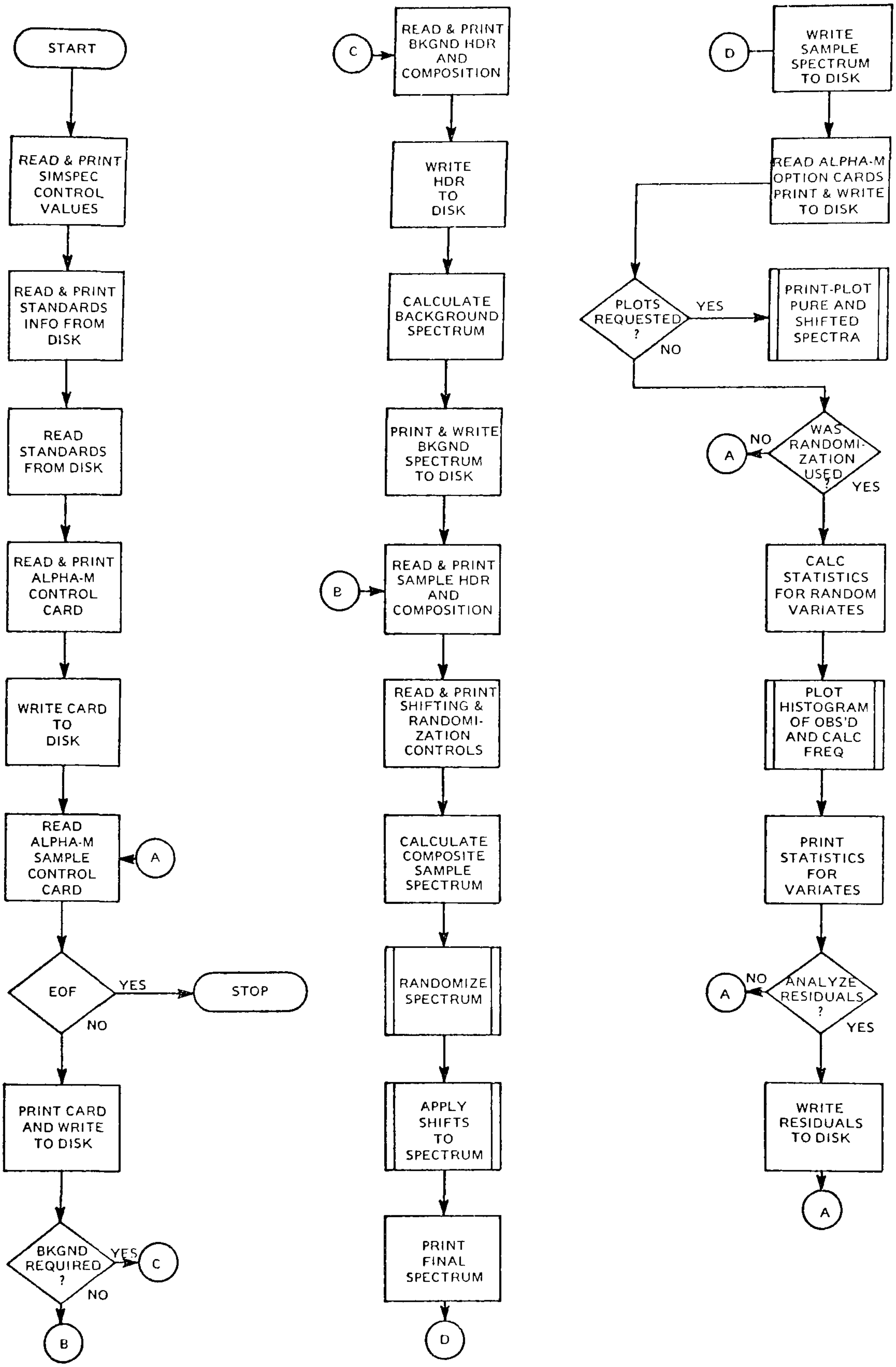

Figure C-2. SIMSPEC flow diagram.

APPENDIX D

TEST DATA

This appendix contains a set of standard spectra for 13 radionuclides (table D-1). These spectra have been stripped of background using a multichannel analyzer. To test ALPHA-M, a standard library can be created from these spectra with GEN4 (table D-2). A background spectrum is included (table D-3).

In addition, two sets of known 3.5-liter water data with the ALPHA-M analysis results also are included. These ALPHA-M analyses were run with the following processing options:

DATA FORMAT 10F7.0
CHANNELS 256
ITERATIONS 5
INITIAL CHANNEL 10
FINAL CHANNEL 181
BKG COUNTING TIME (MINS) 66.67
SAMPLE COUNTING TIME (MINS) 66.67
DECAY TIME 0.0
VOLUME REDUCTION FACTOR 3.5
VOLUME MULTIPLICATION FACTOR 1.0
BKG COMPENSATED AS A LIBRARY STANDARD
WEIGHTS BASED ON RECIPROCAL COUNTS/CHANNEL
AUTOMATIC GAIN & THRESHOLD SHIFT
FULL LIBRARY
NO REJECTION

If these known spectra are run versus the enclosed standard spectra, results similar to those included here should be obtained. The results will not be identical since different processing equipment may have different word size, etc.

TABLE D-1. LIBRARY STANDARDS

(Geometry Type 3.5 Water)

Nuclide	Half-Life (d)	Count Time (Min)	Total Activity (pCi)
^{144}Ce	285.0	66.6666	47396.5
^{51}Cr	27.7	66.6666	20677.0
^{131}I	8.1	66.6666	3941.8
^{106}Ru	365.0	66.6666	17923.9
^{58}Co	71.3	66.6666	5742.4
^{134}Cs	767.0	66.6666	9616.5
^{137}Cs	11100.0	66.6666	16080.0
^{95}Zr	65.0	66.6666	12636.9
^{54}Mn	313.0	66.6666	14366.0
^{65}Zn	245.0	66.6666	16344.6
^{60}Co	1920.0	66.6666	15256.0
^{40}K	999999.0	66.6666	111452.0
^{140}Ba	12.8	66.6666	71167.0
Background	999999.0	66.6666	350.0

TABLE D-2. LIBRARY SPECTRA

Average Background 3.5 Liter Std. Crystal (A) 4/2/75 Stripped

0	0	0	0	12	0	0	0	275	597	594
10	590	595	619	657	701	729	724	717	713	707
20	711	689	681	669	693	706	658	611	589	592
30	577	585	554	524	517	538	556	507	467	405
40	387	368	356	348	354	344	340	346	352	353
50	377	373	382	344	313	278	275	283	292	298
60	303	294	274	248	231	203	195	193	192	184
70	189	176	184	177	176	174	177	165	165	166
80	156	159	159	154	156	151	152	148	141	139
90	140	141	132	129	125	123	115	119	116	115
100	117	115	120	123	122	118	123	113	113	105
110	103	99	99	95	93	94	93	89	91	85
120	87	81	82	80	84	81	82	84	91	94
130	101	100	108	111	107	106	103	92	81	74
140	63	64	59	56	56	51	49	49	54	47
150	48	50	49	52	51	51	52	57	61	57
160	55	55	57	54	51	45	42	41	39	38
170	34	34	33	30	31	30	26	29	28	26
180	28	26	27	25	24	27	25	28	27	29
190	27	28	29	29	33	31	31	38	35	37
200	36	34	33	31	29	27	24	23	19	21
210	20	20	21	16	19	18	18	19	17	19
220	17	17	19	19	17	17	18	20	16	17
230	20	19	19	18	17	16	18	18	16	16
240	16	13	15	13	14	13	13	12	14	12
250	14	13	13	10	12	12				

Ba-La-140 3.5 Liter Std. Crystal (A) 4/2/75 @ 1400 Stripped

0	0	0	18	19	28	24	25	3168	23713	27223
10	31177	35337	37945	39402	41129	42592	45478	53657	55941	47798
20	43824	41894	40326	39610	39072	37990	36799	35188	32963	31915
30	31942	33432	37065	42502	47284	44556	34541	24420	19030	17491
40	17229	17685	18869	21615	22894	23429	24292	28890	38499	48156
50	51917	46600	37722	32648	31908	29717	23911	16682	11770	9394
60	8554	8099	7972	7640	7571	7395	7249	6961	6572	6652
70	6879	7232	8071	8675	9385	10162	11202	13400	16099	18346
80	18897	17362	15296	12280	10390	9473	8814	9123	9183	9151
90	8509	7878	6760	5780	4867	4464	4127	4311	4213	4168
100	4351	4386	4700	4755	4910	4974	5032	4897	4953	4627
110	4676	4670	4762	4732	4799	4849	4976	4809	5055	5134
120	5083	4956	4872	4674	4597	4328	4050	3798	3492	3216
130	2959	2702	2500	2402	2357	2348	2371	2621	2936	3653
140	4736	6298	8435	11535	14727	18340	21068	22339	21725	19590
150	16464	12712	9290	6319	4137	2834	2061	1677	1533	1491
160	1460	1518	1532	1550	1518	1400	1433	1463	1482	1398
170	1337	1315	1210	1141	1203	1202	1260	1232	1164	1093
180	1052	1063	1001	988	1019	1001	1032	1101	1206	1269
190	1264	1272	1239	1224	1053	987	834	723	621 545	
200	481	464	435	408	387	352	351	386	376	433
210	395	456	416	422	449	469	470	552	635	655
220	748	758	813	842	835	835	777	730	690	587
230	490	397	338	248	172	121	57	46	42	7
240	15	7	4	7	7	1	9	2	4	11
250	16	1	1	7	13	13				

TABLE D-2 (cont.)

Ce-144 3.5 Liter Std. Crystal (A) 3/28/75 @ 1130 Stripped

0	4000	0	0	1	1	1	0	4089	9537	9317
10	9591	8714	8069	12016	25719	21239	5162	1342	1143	1093
20	1082	1046	976	982	898	891	836	845	674	698
30	688	617	630	544	547	544	519	561	525	359
40	393	388	307	329	304	279	314	318	284	293
50	278	328	276	215	199	187	157	165	241	229
60	327	314	241	247	276	388	476	683	720	807
70	679	448	325	190	88	72	82	110	67	75
80	97	68	69	17	76	38	71	82	93	93
90	25	97	47	57	74	85	55	43	25	66
100	29	73	26	45	78	67	62	90	74	66
110	62	63	29	72	43	29	56	29	43	38
120	45	34	49	50	12	36	48	55	46	53
130	56	25	26	49	56	62	57	87	68	81
140	63	28	36	51	36	19	26	22	17	21
150	33	39	65	34	54	59	54	50	64	65
160	55	43	47	60	50	24	32	23	23	24
170	39	7	24	39	23	16	17	15	9	12
180	17	8	4	33	16	9	18	5	25	20
190	34	44	65	85	80	90	99	91	78	79
200	70	46	39	14	21	1	3	6	18	7
210	999997	4	999998	999999	999991	4	0	1	5	1
220	3	6	1	999997	999997	999998	5	10	999992	999994
230	7	999996	999997	999989	7	999999	999994	2	999998	999997
240	1	999999	3	6	0	9	999997	5	999996	8
250	2	0	0	999996	2	999999				

Co-58 3.5 Liter Std. Crystal (A) 3/21/75 @ 1525

0	4000	1	0	999999	0	0	1	648	1303	1509
10	1639	1707	2045	2382	2281	2062	1903	2107	2129	2172
20	2363	2616	2575	2661	2399	2314	2117	2075	1920	1742
30	1708	1711	1585	1528	1388	1418	1255	1249	1194	1239
40	1109	1132	1075	1089	1129	1176	1077	1100	1351	1699
50	2360	2922	3247	2941	2136	1463	1067	815	830	716
60	645	592	666	537	442	480	513	436	406	434
70	389	417	499	604	954	1527	2528	3742	4926	5536
80	5131	3962	2608	1372	683	322	153	116	87	90
90	74	112	119	35	97	78	101	100	110	85
100	63	64	51	69	73	71	69	52	106	135
110	103	101	110	78	59	78	67	33	21	38
120	27	69	66	111	156	164	174	143	106	103
130	50	43	13	32	24	33	999980	6	999991	999991
140	13	24	10	999984	7	11	19	22	999995	3
150	29	999996	4	22	0	23	999999	2	26	6
160	999998	999992	999998	7	4	999992	999997	999987	13	999997
170	999992	0	999984	16	3	999996	999992	4	999985	14
180	999999	999998	9	18	2	999992	4	999999	1	3
190	2	999999	4	999999	999998	13	12	17	999986	999995
200	0	5	10	20	999983	8	6	8	3	999995
210	9	0	999992	999991	5	999997	999994	8	1	999994
220	999999	999994	8	3	1	5	6	8	5	999994
230	1	2	4	999999	8	999994	999996	999992	999994	999997
240	6	999994	2	11	0	1	999998	999996	999997	5
250	7	999995	999994	4	2	999996				

TABLE D-2 (cont.)

Co-60 3.5 Liter Std. Crystal (A) 3/17/75 @ 1034

0	4000	1	0	0	1	0	2	1166	3171	3463
10	3767	4139	4311	4889	5248	5270	5366	5261	5282	5303
20	5213	5392	5775	6321	6769	6674	6432	6014	5834	5309
30	5244	4839	4599	4288	4166	3954	3724	3722	3476	3456
40	3453	3213	3048	2988	2968	2878	2864	2889	2799	2780
50	2979	3088	3076	2953	2926	2614	2512	2461	2415	2550
60	2533	2437	2467	2583	2401	2330	2423	2336	2426	2381
70	2520	2462	2459	2619	2598	2735	2747	2640	2649	2529
80	2599	2574	2705	2651	2647	2676	2654	2625	2469	2496
90	2492	2276	2250	2123	2096	1895	1943	1978	1869	1774
100	1783	1888	1809	1914	1994	2269	3262	4061	5573	7137
110	8512	9160	9027	7735	5883	4274	2782	1975	1770	1981
120	2744	3577	4973	6482	7236	7533	7122	6341	4709	3378
130	2121	1337	820	513	338	370	343	336	309	290
140	283	286	298	305	293	267	282	262	278	285
150	280	239	205	217	231	188	207	173	147	137
160	163	178	157	134	192	144	159	136	160	159
170	136	152	153	130	141	129	145	135	145	112
180	141	128	106	127	136	119	122	125	114	123
190	115	138	106	114	101	143	156	125	120	113
200	129	135	119	148	133	115	101	91	106	88
210	84	81	74	64	53	47	44	60	54	59
220	83	99	136	157	193	244	262	250	295	280
230	269	207	198	175	99	77	26	44	21	11
240	5	0	999999	1	999996	999998	5	1	999992	1
250	12	5	11	999998	11	1				

Cr-51 3.5 Liter Std. Crystal (A) 4/1/75 @ 1200 Stripped

0	0	0	1	1	0	0	0	34	616	717
10	813	849	915	927	1019	1327	1574	1550	1276	1056
20	888	876	779	714	638	572	584	639	613	791
30	899	1646	3330	4817	4740	2786	959	230	68	999983
40	118	6	15	999987	4	10	46	30	29	27
50	35	18	999971	6	49	22	19	999953	999989	3
60	72	15	60	34	2	9	999975	30	999986	999990
70	999995	35	999988	33	14	20	999998	999986	26	999985
80	6	24	10	999972	33	11	999997	26	6	999993
90	21	999992	7	999975	999995	21	3	14	10	999992
100	999992	13	12	999998	1	25	999989	17	12	11
110	999981	21	999995	6	999983	10	19	999966	999991	2
120	20	9	999992	13	4	9	14	9	999996	5
130	19	14	32	999995	999995	21	999980	20	999992	999988
140	9	7	999992	999996	8	11	999995	0	5	20
150	15	5	1	999997	999992	999980	999996	18	7	16
160	4	999992	999999	23	11	999993	1	7	999987	999999
170	999998	20	10	999985	999991	999994	999995	999991	999999	999996
180	999998	999991	999998	7	999994	4	1	2	999996	4
190	999999	1	3	999998	999997	999983	999991	999992	4	999991
200	7	13	999987	3	13	999997	5	999996	999997	999994
210	999995	0	1	999996	999998	999997	6	999993	999992	4
220	0	999995	999999	999996	6	3	999988	999998	999997	2
230	999998	999997	3	999984	1	9	1	999996	999989	2
240	999996	999993	999984	5	999998	999989	2	7	999990	0
250	2	6	999994	999996	6	999997				

TABLE D-2 (cont.)

Mn-54 3.5 Liter Std. Crystal (A) 3/20/75 @ 1021

0	4000	2	0	3	0	0	1	798	2223	2493
10	2682	2867	3372	3571	3627	3925	3748	3701	3783	3946
20	4198	4695	5096	5257	4724	4622	4287	3969	3738	3629
30	3329	3108	3028	2914	2728	2586	2567	2506	2352	2497
40	2261	2358	2223	2279	2236	2129	2031	2114	2002	2184
50	2141	2168	2029	2112	2083	2093	2059	2180	2108	2167
60	1879	1702	1652	1426	1316	1134	1035	914	922	861
70	778	801	840	762	866	1317	1909	3443	5599	8659
80	12222	14226	14259	12266	8360	4836	2185	841	277	65
90	999979	999981	12	3	999964	999975	3	999988	2	4
100	999971	999985	999978	999969	999995	999991	999999	999977	999985	999978
110	999991	999970	999983	999995	999978	999980	999997	999989	999982	6
120	999985	999998	9	999986	8	999983	10	999987	999994	999998
130	999983	999965	999969	999978	6	999976	4	28	6	1
140	28	8	19	999992	999995	2	14	4	1	16
150	999997	999984	6	999984	999987	999994	999993	3	999995	999996
160	10	999991	999975	5	999987	999998	999986	1	999998	4
170	999997	0	999997	999995	999990	0	2	6	6	999991
180	999996	1	999998	2	4	999988	12	999990	999998	999991
190	999987	6	999993	2	1	999986	5	5	999989	999980
200	999999	999992	999988	999984	999993	7	999998	1	4	999994
210	999996	2	999992	999989	7	1	2	4	999995	7
220	9	999994	0	999997	12	3	999990	999999	4	5
230	999985	999992	999997	999993	0	1	999986	999997	2	999998
240	999995	9	999982	4	999997	999991	999987	999997	7	999997
250	999995	1	5	999999	8	3				

Cs-134 3.5 Liter Std. Crystal (A) 3/18/75 @ 1632

0	4000	4	0	0	2	1	999999	1505	3835	4251
10	4628	5022	5460	6017	6411	6377	6175	6326	6483	7197
20	7953	8457	8528	7894	7470	7146	6580	6091	5748	5437
30	5240	4927	4923	4633	4610	4357	4296	4129	4166	4118
40	3939	3782	3744	3481	3195	3203	3168	3211	3277	3203
50	3176	3128	3113	3172	3667	4134	5217	6754	8381	10213
60	11703	11591	9225	5984	3442	1778	1335	1246	1374	1787
70	2404	3125	4403	5656	7282	8733	9766	10168	9408	7692
80	5610	3434	1995	1083	640	524	477	444	507	457
90	438	458	427	442	456	454	511	450	484	453
100	416	425	384	385	337	352	317	302	367	351
110	395	430	431	392	398	293	242	216	188	159
120	141	171	119	149	152	219	257	302	341	392
130	410	445	470	539	488	393	345	224	150	99
140	53	44	25	29	999999	25	14	8	17	12
150	8	25	10	10	24	16	17	44	9	26
160	17	999981	11	999997	19	5	3	999995	12	999996
170	1	15	9	15	999988	7	7	17	0	10
180	0	30	16	21	15	12	24	20	6	999999
190	0	999989	19	999993	999999	6	999995	1	4	999989
200	999995	999996	7	999986	999991	2	10	5	999999	999995
210	999999	999986	999988	1	999993	12	999997	999998	0	0
220	6	10	999997	11	2	999996	999997	999996	0	1
230	5	9	3	999998	7	0	999997	1	999999	6
240	999997	5	3	0	2	999998	8	999999	999989	999996
250	999990	4	1	7	1	3				

TABLE D-2 (cont.)

Cs-137 3.5 Liter Std. Crystal (A) 3/19/75 @ 1409

0	4000	0	0	1	999999	0	0	990	2368	2787
10	2938	3159	3612	3814	4058	4072	4038	4068	4191	4600
20	5031	5426	5652	5017	4869	4263	4082	3939	3657	3475
30	3282	3109	3010	2730	2762	2592	2592	2655	2495	2502
40	2433	2441	2462	2456	2436	2355	2192	1991	1709	1440
50	1418	1251	1193	1200	1067	1072	1013	1043	1077	1159
60	1476	2290	4050	7293	11120	14640	16272	14298	9706	5216
70	2095	600	117	4	6	21	999995	999985	14	999972
80	999996	30	999983	12	999995	999994	40	999994	999985	32
90	17	10	28	999997	7	11	36	19	41	7
100	10	11	999973	999985	999985	999990	999993	19	999992	4
110	10	3	14	1	2	15	999995	999991	999989	10
120	999992	999984	5	999991	4	999982	0	7	4	999987
130	29	3	0	999978	23	25	999996	3	2	999993
140	999997	4	999984	999999	1	19	999992	9	999995	1
150	999984	999996	999999	999979	999995	20	999995	0	999993	999983
160	12	6	1	999992	2	9	10	6	11	999998
170	3	3	999990	999997	2	999994	13	1	999990	999996
180	5	999987	3	7	0	19	999990	999993	999991	999992
190	5	4	4	999997	999991	999990	2	999979	999995	6
200	999993	999993	10	3	999989	999993	18	11	9	0
210	10	999992	999988	6	999999	999996	999994	7	999999	3
220	2	0	999988	8	999995	11	999991	999997	12	4
230	999999	999995	999998	999997	999998	1	999999	1	999998	999996
240	999995	999996	999999	999992	2	3	10	999998	999992	3
250	999987	3	999996	999997	999988	3				

I-131 3.5 Liter Std. Crystal (A) 3/24/75 @ 1543

0	4000	1	1	1	0	0	0	549	1432	1302
10	1409	1693	1660	1814	1881	1935	2264	2612	2556	2376
20	2252	2028	1847	1629	1373	1300	1239	1248	1332	1532
30	1637	1539	1167	1128	1270	1836	3752	5943	7072	5903
40	3225	1185	343	157	130	169	157	172	213	246
50	404	449	525	538	333	180	133	139	46	145
60	223	327	521	521	510	323	222	145	112	105
70	109	221	203	195	241	292	222	202	119	2
80	52	7	3	25	29	19	33	31	999983	49
90	10	49	15	17	7	15	999996	16	12	49
100	11	33	999997	8	999994	6	47	33	22	42
110	0	0	12	41	10	0	13	19	23	999994
120	6	6	7	999993	0	4	22	17	17	31
130	7	15	16	7	4	999990	999995	.999990	999984	999991
140	12	999975	999992	1	12	999991	999989	1	5	0
150	19	999992	11	999998	999994	999984	999992	3	999984	13
160	999996	9	999993	19	15	7	999993	999993	1	2
170	18	999996	999993	17	12	13	15	11	999981	999991
180	999996	999993	21	999995	0	999989	0	4	3	10
190	7	6	999997	999998	8	21	5	999998	16	12
200	6	999996	999995	999986	1	999998	999994	4	7	1
210	999997	999999	9	1	1	999994	8	7	8	3
220	1	999999	1	6	999999	3	999995	999995	999990	8
230	3	3	3	999989	5	5	999996	999995	999999	999996
240	999996	8	0	999997	3	1	999989	999997	3	999992
250	999999	1	999999	8	999997	4				

TABLE D-2 (cont.)

K-40 3.5 Liter Std. Crystal (A) 3/27/75 @ 1331

0	4000	0	0	0	0	0	1	1161	2433	2423
10	2627	2651	2754	2791	2733	2793	2754	2693	2589	2515
20	2439	2446	2440	2469	2717	2796	2750	2629	2419	2225
30	2063	2149	1897	1803	1804	1609	1508	1402	1422	1329
40	1172	1223	1210	1144	1158	1128	1065	1158	1009	1072
50	1203	1280	1397	1276	1168	980	891	838	846	821
60	867	929	919	818	862	818	778	775	750	823
70	747	792	783	829	931	962	911	829	823	730
80	826	777	766	746	722	759	730	741	731	789
90	811	808	839	867	889	828	845	866	841	857
100	972	896	868	903	975	929	901	981	980	977
110	982	928	888	812	770	674	585	527	472	397
120	350	352	346	342	358	386	406	537	811	1097
130	1594	2351	3193	4032	4877	5240	5130	4495	3744	2614
140	1688	975	519	226	98	51	26	7	6	20
150	8	999990	6	999979	18	0	9	999999	999996	999997
160	3	0	999995	12	999995	22	999995	999996	999993	999999
170	17	0	16	6	999997	999985	10	14	6	0
180	999993	999996	14	1	13	999993	1	999990	3	8
190	999998	5	999999	999988	999980	4	13	7	999999	999994
200	999999	3	3	1	999985	6	3	5	1	999999
210	999996	7	4	4	999997	999996	3	999989	2	4
220	8	4	6	999997	999990	7	999998	6	8	999996
230	2	1	999996	999994	1	999997	1	15	999998	1
240	8	999998	3	3	999995	0	999996	1	999990	999993
250	999990	4	999997	4	6	7				

Ru-106 3.5 Liter Std. Crystal (A) 3/20/75 @ 1513

0	4000	0	0	0	1	0	0	975	2182	2455
10	2588	2747	2994	3089	2950	2983	3000	2980	3120	3429
20	3635	3644	3457	3243	2983	2677	2460	2335	2156	2219
30	1990	1895	1965	1797	1669	1544	1425	1309	1312	1264
40	1251	1258	1221	1174	1117	1153	1019	1174	1541	2460
50	4098	6165	7350	6929	4702	2466	1164	606	704	1034
60	1672	2319	2836	2819	2212	1378	826	459	283	202
70	221	239	245	203	239	238	187	216	251	196
80	187	211	249	274	233	201	234	197	170	151
90	135	114	162	135	104	82	93	163	206	232
100	277	265	211	236	234	181	133	188	209	242
110	293	258	205	183	123	77	68	20	4	40
120	19	999994	25	20	21	10	47	7	7	12
130	7	14	31	999982	19	9	11	36	5	15
140	24	18	48	13	13	58	26	35	27	45
150	20	22	28	999989	3	999997	999998	29	3	11
160	15	7	999989	22	999993	7	999988	9	1	5
170	7	4	999997	999988	11	4	1	11	13	1
180	999995	999999	3	5	999998	999982	13	999999	3	999990
190	2	9	7	999994	11	999989	0	24	999997	999995
200	999989	999994	999985	999995	6	1	3	999996	10	999995
210	999996	999992	999999	5	4	15	7	14	999998	999998
220	12	999999	6	999999	23	0	999992	999999	2	5
230	999994	999990	999993	999993	4	8	999988	1	6	4
240	999999	18	999991	6	999997	999992	999984	3	2	5
250	999989	6	1	3	999998	999997				

TABLE D-2 (cont.)

Zn-65 3.5 Liter Std. Crystal (A) 3/24/75 @ 1022

0	4000	0	0	0	1	2	2	421	1289	1376
10	1633	1633	1853	2082	2175	2232	2097	2305	2209	2328
20	2204	2443	2657	2920	2901	2791	2710	2614	2303	2180
30	2174	1977	1812	1788	1597	1588	1587	1461	1448	1390
40	1277	1288	1233	1170	1224	1206	1164	1264	1240	1417
50	1608	1904	2019	1850	1527	1190	1062	988	926	951
60	1029	954	973	1029	943	1023	962	990	1005	1062
70	1001	1093	1055	1051	1042	1065	1094	1102	1145	1090
80	1122	1204	1138	972	994	859	790	719	588	542
90	486	502	393	382	359	387	406	466	547	803
100	1204	1872	2904	4091	5596	6582	7378	6763	5560	4100
110	2537	1387	707	285	102	49	15	8	0	999989
120	7	999995	18	22	2	14	999996	14	999995	23
130	999985	7	5	999991	999990	999998	999996	999984	0	7
140	10	999982	2	999983	3	5	10	1	8	1
150	19	999984	3	1	999995	999970	999975	17	999990	999996
160	999993	1	999978	24	4	3	999989	999995	999996	0
170	7	5	999993	9	20	999998	1	7	999995	999985
180	999989	999994	11	1	0	999982	1	999996	999986	999998
190	5	999997	999999	999996	7	999998	999995	3	999999	999999
200	1	2	999991	999992	999997	999995	999999	0	4	2
210	999990	999998	13	4	5	999996	16	999989	999999	5
220	9	0	999999	11	999998	6	999995	3	999990	3
230	999995	999994	7	999993	7	12	999999	999998	999995	999999
240	1	2	3	4	1	999993	999988	6	3	999996
250	4	8	999998	999997	999996	0				

Zr-95 3.5 Liter Std. Crystal (A) 3/31/75 @ 1309

0	4000	1	1	1	0	0	0	868	2010	2262
10	2402	2698	2891	3234	3345	3383	3453	3381	3501	3583
20	3910	4498	4603	4621	4312	4018	3815	3547	3272	3080
30	2909	2767	2700	2591	2419	2324	2273	2160	2087	2053
40	2095	2038	1953	1981	1968	1955	1868	2076	2063	1933
50	1930	2046	1864	1882	1850	1616	1366	1241	1057	946
60	892	940	816	811	797	821	847	1153	1414	2229
70	3434	5254	7320	9363	11380	11677	10364	7660	4627	2109
80	856	265	25	19	999981	11	8	999988	29	12
90	21	20	999990	21	999992	999991	16	3	999998	11
100	999997	7	9	999990	999992	9	999993	14	999958	999979
110	27	3	999991	9	1	999988	999991	9	999987	10
120	999995	999984	999986	4	999980	11	5	12	15	999981
130	999997	999999	7	999977	28	999985	11	13	999981	0
140	24	999991	999992	999995	14	1	1	18	999994	12
150	17	10	1	6	999995	16	999999	3	10	11
160	999993	19	10	999993	999993	999983	999993	4	999987	12
170	14	1	2	3	5	999995	2	16	2	6
180	8	999996	999995	999981	3	999997	999998	999989	999990	999991
190	999995	999996	13	0	6	999996	999989	999995	9	999997
200	7	8	6	999997	4	999993	6	999995	999992	14
210	2	7	999997	1	3	0	5	4	5	9
220	7	4	999999	5	6	7	4	999989	2	10
230	999993	3	10	7	1	0	5	3	4	9
240	2	999997	999995	0	5	0	12	999994	2	3
250	3	999992	999986	6	11	999994				

TABLE D-3. TEST SPECTRA

100 PCI/LITER CS-137 + BACKGROUND

1.0	784149.1	0.0	18.3	0.1	0.0	0.0	304.1	625.1	639.0
659.1	692.5	694.2	712.9	801.4	811.5	794.8	794.9	793.2	825.5
814.6	834.2	776.1	745.1	749.4	783.0	768.7	658.5	658.6	677.6
582.8	671.1	610.1	596.1	613.4	624.0	621.0	583.2	481.1	448.1
459.6	460.9	445.5	394.4	394.2	378.0	404.6	356.7	400.6	394.3
368.0	394.0	421.9	353.8	358.7	297.2	300.3	312.0	299.5	292.8
356.4	348.0	354.7	407.1	458.4	520.2	539.1	495.6	395.2	276.2
248.3	226.4	197.2	175.5	162.1	196.9	181.0	183.8	174.6	170.0
144.8	172.3	153.0	153.5	150.3	168.7	159.5	133.1	136.4	126.7
144.3	133.3	144.7	117.2	134.0	122.0	110.1	98.3	127.7	126.9
119.5	106.3	124.5	121.3	117.5	105.2	146.5	96.7	107.3	110.1
104.3	97.8	110.3	95.0	85.7	103.7	90.6	95.9	112.6	72.1
76.1	74.9	90.3	87.4	86.0	76.7	78.7	98.4	103.5	99.2
100.7	85.4	105.1	117.9	113.1	107.9	92.3	108.9	82.6	69.7
55.3	66.6	64.0	50.2	40.5	55.5	46.5	50.7	57.1	44.9
56.2	41.7	51.3	56.6	56.0	49.7	36.4	44.4	52.0	55.0
57.9	59.3	42.9	52.3	39.5	48.9	34.6	32.1	28.4	36.7
28.6	32.7	30.9	29.9	30.6	22.4	27.0	27.6	33.0	24.5
22.8	39.7	31.0	15.7	28.5	22.6	36.1	27.4	34.2	31.2
25.8	29.9	28.8	34.9	28.1	38.1	30.1	28.6	20.1	39.3
34.6	41.9	30.8	27.9	27.0	31.7	17.5	27.4	18.6	17.5
23.4	26.6	13.4	14.1	23.6	19.3	11.6	25.9	16.7	14.4
25.6	20.1	19.4	21.5	20.4	14.1	12.8	15.4	14.2	19.6
16.4	13.8	17.2	18.0	17.3	17.0	19.9	12.6	15.6	19.0
16.4	12.7	15.4	10.4	10.1	14.8	14.6	12.2	15.7	14.4
21.2	10.8	16.4	6.9	7.4	10.5				

BACKGD SUM= 38585. SAMPLE SUM= 43577.

TABLE D-3 (cont.)

SAMPLE NUMBER 1 ID NO. CS - 137 ... PROCESSING OPTION NUMBER 1

BACKGROUND WILL NOT BE SUBTRACTED THIS OPTION
WEIGHTS TO BE BASED ON CALCULATED SAMPLE SPECTRUM
WEIGHTS PROPORTIONAL TO RECIPROCAL COUNTS/CHANNEL
NO REJECTION COEFFICIENT APPLIED
AUTOMATIC COMPENSATION REQUIRED FOR GAIN AND THRESHOLD SHIFT
NUMBER OF ISOTOPES USED FROM LIBRARY IS 14
THRESHOLD CHANNEL SHIFT BETWEEN STDS AND SAMPLE IS 0.0
LIBRARY STD. NUMBERS, IN ORDER OF DESIRED OUTPUT ARE 1 2 3 4 5 6 7 8 9 10 11 12 13 14
NORMALIZED RESIDUALS WILL NOT BE PLOTTED
OBSERVED AND CALCULATED SPECTRA WILL NOT BE PLOTTED
MATRIX INFORMATION WILL NOT BE PRINTED

CHDF = 0.51 THR SHIFT = -0.0827 GAIN SHIFT = 1.0006
CHDF = 0.47 THR SHIFT = -0.1061 GAIN SHIFT = 1.0007
CHDF = 0.46 THR SHIFT = -0.1119 GAIN SHIFT = 1.0008
CHDF = 0.45 THR SHIFT = -0.1129 GAIN SHIFT = 1.0007
CHDF = 0.45 THR SHIFT = -0.1127 GAIN SHIFT = 1.0007

LIBRARY NUMBER	NUCLIDE NAME	DECAY UNCORRECTED ACTIVITY	DECAY UNCORRECTED STD. ERR.	DECAY CORRECTED ACTIVITY	DECAY CORRECTED STD. ERR.	COEFFICIENT OF VARIANCE	ALPHA FACTOR	LLD
1	CE-144	8.0393	10.8042	8.0393	10.8042	134.39	0.5994	35.5457
2	CR-51	37.8064	18.1012	37.8064	18.1012	47.88	0.6750	59.5528
3	I-131	0.6294	2.3406	0.6294	2.3406	371.90	0.9629	7.7006
4	RU-106	5.2724	8.5739	5.2724	8.5739	162.62	1.4086	28.2080
5	CO-58	-2.2279	3.8864	-2.2279	3.8864	174.44	1.7700	12.7862
6	CS-134	3.0924	2.5749	3.0924	2.5749	83.27	2.1799	8.4715
7	CS-137	97.2948	3.2677	97.2948	3.2677	3.36	0.9410	10.7506
8	ZR-NB-95	2.3822	2.9046	2.3822	2.9046	121.93	0.9827	9.5563
9	MN-54	1.5687	2.8453	1.5687	2.8453	181.38	1.0022	9.3611
10	ZN-65	-0.5341	3.2912	-0.5341	3.2912	616.24	0.6935	10.8279
11	CO-60	4.0074	1.6393	4.0074	1.8393	45.90	1.0862	6.0512
12	K-40	43.4119	28.7280	43.4119	28.7280	66.18	0.9498	94.5150
13	BA-140	2.6267	2.8958	2.6267	2.8958	110.24	1.9728	9.5270
14	BACKGRND	94.4244	2.0989	94.4244	2.0989	2.22	4.5156	6.9053

NORMALIZED RESIDUALS PER CHANNEL

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.2	0.3	0.9	0.0	-0.5	0.2	-0.3	-0.4	-0.2	-0.1	0.6
0.1	0.7	-0.6	-0.7	-1.0	-0.2	0.5	-0.9	-0.0	0.2	-1.5	0.4	-0.6	-0.2	0.5	0.7	0.3	0.6	-1.1	-0.1
0.9	1.6	1.4	0.0	-0.2	-0.3	0.8	-0.8	0.6	0.4	-1.2	-0.1	0.4	-0.5	0.7	-0.1	0.2	0.3	-0.6	-1.1
0.7	0.0	-0.2	0.3	-0.1	0.4	-0.0	-0.1	-0.2	-0.8	0.7	1.8	0.3	-0.5	-1.2	0.5	-0.3	0.5	0.2	0.0
-0.6	0.6	-0.4	-0.1	-0.2	1.1	0.5	-0.7	-0.1	-0.6	0.4	-0.2	0.9	-0.5	0.7	0.0	-0.2	-1.1	0.9	1.0
0.3	-0.4	0.5	0.1	-0.1	-0.6	1.6	-1.0	-0.4	0.1	-0.3	-0.4	0.4	-0.3	-0.7	0.6	-0.1	0.7	1.7	-0.9
-0.8	-0.4	0.5	0.4	-0.1	-0.6	-0.5	0.9	0.8	0.4	-0.0	-1.0	-0.2	0.4	0.2	-0.1	-0.9	1.0	-0.0	-0.4
-0.6	0.3	0.6	-0.5	-1.4	0.4	-0.3	0.0	0.3	-0.3	0.9	-0.7	0.3	0.7	0.7	0.1	-1.3	-0.9	-0.5	0.1
0.5	0.7	-1.1	0.1	-0.9	0.6	-0.6	-0.8	-1.0	0.0	-0.5	0.1	-0.1	0.2	0.1	-0.8	0.2	0.0	0.9	-0.1
-0.5																			

AVERAGE =-0.0068 STD. DEV. = 0.6414 SKEWNESS = 0.1628 KURTOSIS = 2.8257
PERCENT OF RESIDUALS UNDER 1 SIGMA = 66.9 2 SIGMA = 95.3 3 SIGMA =100.0

SAMPLE/OPTION WRITTEN TO IOPT AT 05/27/76 17:02:49

TABLE D-3 (cont.)

CONTROL INFORMATION ..... SAMPLE NUMBER 2   SAMPLE ID IS: CO - 60

NUMBER OF PROCESSING OPTIONS IS 1
COUNTING TIME (MINS.) FOR BKGND IS 66.67
COUNTING TIME (MINS.) FOR SAMPLE IS 66.67
DECAY TIME (DAYS) IS 0.0
VOLUME REDUCTION FACTOR IS 3.500
VOLUME MULTIPLICATION FACTOR IS 1.000
SAMPLE TIME/BKGND TIME = FS = 1.000
VALUE OF FS**2 = FX = 1.000
SAMPLE BACKGROUND NOT INPUT; PREVIOUS BKGND WILL BE USED IF SUBTRACTION REQUESTED
PERMANENT BACKGROUND SUBTRACTION NOT REQUESTED
DETECTOR A STANDARDS SELECTED

100 PCI/LITER CO-60 + BACKGROUND

1.0	785797.6	0.0	7.6	-0.2	0.0	-0.1	284.1	679.3	704.4
704.3	692.2	691.9	732.0	819.8	849.8	862.1	855.5	839.6	838.5
804.2	790.3	827.6	781.5	832.6	892.9	769.0	726.8	723.1	690.7
687.8	698.6	664.8	636.7	601.9	655.9	611.6	628.6	504.7	492.6
444.5	421.2	398.2	410.9	412.1	417.0	421.6	398.1	425.8	407.6
440.5	427.7	462.3	437.7	404.2	361.6	362.8	336.8	328.4	361.1
372.2	367.9	370.3	314.6	268.2	273.8	244.2	235.0	249.3	227.6
246.2	250.5	217.7	270.7	240.2	234.4	247.6	227.1	223.0	207.6
198.8	209.5	196.2	223.5	237.5	201.0	233.4	205.1	202.7	188.9
182.4	202.8	184.5	157.5	173.8	161.2	159.2	167.7	158.8	156.1
174.4	172.6	153.9	156.6	162.1	174.9	179.5	212.6	266.5	260.8
293.3	331.5	313.1	256.0	191.1	188.1	161.1	134.8	115.3	131.5
169.6	165.4	185.8	195.6	263.5	268.2	237.2	217.5	158.3	179.3
149.1	125.0	122.5	142.8	109.8	111.6	94.0	124.5	89.3	90.6
64.4	70.6	61.9	58.4	66.2	50.8	53.0	71.4	64.1	68.3
49.0	58.1	53.9	58.6	52.1	67.9	47.4	70.0	55.1	71.1
70.2	53.0	55.8	64.0	46.2	46.0	41.2	45.8	48.1	51.1
44.0	40.0	41.9	30.0	38.2	27.8	33.5	31.3	29.4	31.8
39.6	29.4	19.7	28.2	26.2	40.0	27.8	28.5	30.3	32.4
26.7	39.9	37.2	35.3	35.5	27.3	33.7	38.9	42.4	41.7
46.5	42.8	34.8	28.0	23.9	29.8	19.9	21.2	17.6	20.1
18.9	21.3	19.8	21.3	12.1	14.1	22.2	15.2	26.9	25.9
22.7	17.2	14.8	22.3	20.5	19.8	24.1	32.0	15.5	20.8
30.6	18.9	24.9	26.8	25.7	10.7	14.0	14.2	16.5	18.0
13.5	12.6	12.5	8.1	11.7	15.9	6.4	11.8	14.5	12.4
11.9	13.0	15.9	12.3	4.9	8.7				

BACKGD SUM= 38585.   SAMPLE SUM= 49153.

SAMPLE NUMBER 2 ID NO. CO - 60 ... PROCESSING OPTION NUMBER 1

BACKGROUND WILL NOT BE SUBTRACTED THIS OPTION
WEIGHTS TO BE BASED ON CALCULATED SAMPLE SPECTRUM
WEIGHTS PROPORTIONAL TO RECIPROCAL COUNTS/CHANNEL
NO REJECTION COEFFICIENT APPLIED
AUTOMATIC COMPENSATION REQUIRED FOR GAIN AND THRESHOLD SHIFT
NUMBER OF ISOTOPES USED FROM LIBRARY IS 14
THRESHOLD CHANNEL SHIFT BETWEEN STDS AND SAMPLE IS 0.0
LIBRARY STD. NUMBERS, IN ORDER OF DESIRED OUTPUT ARE 1 2 3 4 5 6 7 8 9 10 11 12 13 14
NORMALIZED RESIDUALS WILL NOT BE PLOTTED
OBSERVED AND CALCULATED SPECTRA WILL NOT BE PLOTTED
MATRIX INFORMATION WILL NOT BE PRINTED

CHDF = 0.56 THR SHIFT = -0.2784 GAIN SHIFT = 1.0025
CHDF = 0.45 THR SHIFT = -0.4248 GAIN SHIFT = 1.0038
CHDF = 0.42 THR SHIFT = -0.4749 GAIN SHIFT = 1.0043
CHDF = 0.41 THR SHIFT = -0.4891 GAIN SHIFT = 1.0045
CHDF = 0.40 THR SHIFT = -0.4935 GAIN SHIFT = 1.0046

LIBRARY	NUCLIDE	DECAY UNCORRECTED		DECAY CORRECTED		COEFFICIENT	ALPHA	
NUMBER	NAME	ACTIVITY	STD. ERR.	ACTIVITY	STD. ERR.	OF VARIANCE	FACTOR	LLD
1	CE-144	11.9322	10.6853	11.9322	10.6853	89.55	0.6775	35.1546
2	CR-51	7.3103	16.1592	7.3103	16.1592	221.05	0.6886	53.1637
3	I-131	-4.9429	2.3205	-4.9429	2.3205	46.95	1.0910	7.6345
4	RU-106	12.3069	7.9590	12.3069	7.9590	64.67	1.4943	26.1852
5	CO-58	-9.4041	3.6858	-9.4041	3.6858	39.19	1.9184	12.1263
6	CS-134	3.2343	2.2285	3.2343	2.2285	68.90	2.1560	7.3319
7	CS-137	-2.3154	2.1345	-2.3154	2.1345	92.19	0.7025	7.0226
8	ZR-NB-95	1.7026	2.7418	1.7026	2.7418	161.04	1.0601	9.0205
9	MN-54	1.8644	2.8731	1.8644	2.8731	154.10	1.1565	9.4527
10	ZN-65	0.8855	3.9634	0.8855	3.9634	447.61	0.9544	13.0396
11	CO-60	96.9404	2.4410	96.9404	2.4410	2.52	1.6474	8.0310
12	K-40	23.1337	26.7016	23.1337	26.7016	115.42	1.0088	87.8484
13	BA-140	4.0530	2.7504	4.0530	2.7504	67.86	2.1414	9.0487
14	BACKGRND	98.2321	2.0010	98.2321	2.0010	2.04	4.9198	6.5833

NORMALIZED RESIDUALS PER CHANNEL

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.5	-0.0	-0.3	-0.2	-0.2	-0.2	0.3	0.4	0.2	0.0
-0.7	-0.2	0.1	-0.2	0.1	-0.1	-1.2	-0.6	-0.2	-0.5	-0.0	-0.1	-0.2	0.0	-0.0	0.5	-0.4	0.8	-0.5	0.7
-0.5	-0.8	-0.8	-0.2	-0.3	0.3	0.4	-0.3	0.1	-0.2	-0.4	-0.5	-0.0	0.5	0.4	0.7	0.8	-0.3	-0.7	-0.0
-0.0	0.2	0.8	-0.2	-0.6	0.9	0.0	-0.0	0.2	-0.3	-0.0	0.5	-0.9	1.1	-0.2	-0.3	0.2	0.3	0.4	-0.0
0.0	0.1	-0.8	0.6	0.9	-0.4	0.9	-0.1	0.2	-0.4	-0.7	0.5	0.0	-1.0	0.0	-0.3	0.1	0.2	0.0	0.1
1.0	0.8	-0.5	-0.5	-0.4	0.3	-1.0	0.4	1.4	-0.2	-0.1	1.3	0.6	-0.6	-1.8	-0.1	1.6	0.2	-1.0	0.1
1.2	0.3	-0.5	-1.7	0.7	1.1	-0.0	-0.3	-1.9	0.5	0.2	-0.2	-0.4	1.0	-0.3	-0.4	-1.2	1.3	0.2	0.7
-0.2	-0.2	-0.3	-0.5	0.1	-0.6	-0.6	0.9	0.1	1.0	-0.4	-0.1	-0.1	0.0	-0.3	1.0	-0.5	0.5	-0.5	0.7
1.2	-0.2	-0.4	0.5	-0.4	-0.2	-0.3	0.1	0.6	1.0	1.0	0.5	0.6	0.1	0.3	-0.3	0.4	0.0	-0.1	0.3
0.8																			

AVERAGE = 0.0352 STD. DEV. = 0.6036 SKEWNESS = 0.0630 KURTOSIS = 3.5627
PERCENT OF RESIDUALS UNDER 1 SIGMA = 71.5 2 SIGMA = 94.8 3 SIGMA = 98.8

SUSPICIOUS CHANNELS

-115 -129

SAMPLE/OPTION WRITTEN TO IOPT AT 05/27/76 17:02:50

* * * * * * * ALPHA-M NORMAL TERMINATION * * * * * * *

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/7-77-089	2.	3. RECIPIENT'S ACCESSION NO.
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15. SUPPLEMENTARY NOTES

This project is part of the EPA-planned and coordinated Federal Interagency Energy/Environment R&D Program.

16. ABSTRACT

The use of ALPHA-M, a least-squares computer program for analyzing NaI (Tℓ) gamma spectra of environmental samples, is evaluated. Included is a comprehensive set of program instructions, listings, and flowcharts. Two other programs, GEN4 and SIMSPEC, are also described. GEN4 is used to create standard libraries for ALPHA-M, and SIMSPEC is used to simulate spectra for ALPHA-M analysis. Tests to evaluate the standard libraries selected for use in analyzing environmental samples are provided. An evaluation of the results of sample analyses is discussed.

17. (Circle One or More) KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS			b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Ecology	Hydrology, Limnology	Energy Conversion		6F 8A 8F
Environments	Biochemistry	Physical Chemistry		8H 10A 10B
Earth Atmosphere	Earth Hydrosphere	Materials Handling		7B 7C 13B
Environmental Engineering	Combustion	Inorganic Chemistry		
Geography	Refining	Organic Chemistry		
		Chemical Engineering		
Other:				

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