NUS - 282

First Quarterly Report

for

Project CUBED

A Code to Unfold Bremsstrahlung Experimental Distributions

(13 January, 1966 - 13 April, 1966)

Contract No.: NAS5 - 10133

Prepared by

Julian J. Steyn
Technical Associate

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Goddard Space Flight Center

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SUMMARY

This report discusses the initial development of a FORTRAN IV IBM-7094 digital computer code to unfold bremsstrahlung photon distributions recorded by a sodium-iodide scintillation spectrometer. The code--CUBED--is described in some detail. A system response matrix is generated from the characteristic spectra of standard radioisotope sources and applied to compute the incident photon number distribution by the Scofield iterative unfolding technique. The code executes anciliary analysis such as determination of energy differential spectra, energy integrated number, energy and dose data. The code description is preceded by a short theoretical background discussion. CUBED makes use of certain existing codes; these are delineated.

The future status of the code, presently in the preliminary testing stage, is discussed. The work program required to complete the code development is reviewed.

1. INTRODUCTION

This first quarterly report discusses the initial development of a digital computer code to semi-automatically unfold continuous gamma photon scintillation spectra. The continuous spectra for which the code is specifically intended are those recorded by the right-cylindrical sodium-iodide (thallium activated)--NaI(Tl)--scintillation crystal, coupled to a multi-channel pulse-height analyzer and exposed to the bremsstrahlung photon field generated by right-cylindrical beta emitting isotopic sources.

The emission of beta radiation by isotopic sources of finite extent is accompanied by the generation within the source domain of continuous or polyenergetic, electromagnetic radiation known as bremsstrahlung.[1] In order to carry out an experimental spectrometric analysis of the extent of bremsstrahlung emitted by beta sources, it is a first prerequisite to develop a method of reducing the spectrometer measured spectra to photon number spectra. The analysis must recognize the limited resolution and nonunique pulse-height response of the scintillation spectrometer to monoenergetic photons and, thus, account for its response to polyenergetic photon distributions. The analysis should also include such factors as primary source decay, conversion of photon number spectra to photon energy spectra and total exposure dose, the subtraction of background radiation, and the normalization of results to units convenient for subsequent further analysis.

A review of existing methods[2-7] of analyzing continuous scintillation photon spectra indicated the Scofield iterative unfolding method,[7] employing an experimentally determined spectrometer system response matrix, to be most amenable to the task at hand. With this method the unfolding process may be considered as two operations:

(1) Generation of the system response matrix

(2) Iterative unfolding (Scofield method).

During the present report period--CUBED--a digital computer Code to Unfold Bremsstrahlung Experimental Distributions has been developed. This code, written in the FORTRAN IV language for the IBM-7094 computer and presently in the initial testing stage, will generate the system response matrix employing standard spectra and iteratively unfold continuous spectra to yield photon number spectra. It will also

correct for primary source decay, radiation background, compute energy spectra and exposure dose and order data for further analysis.

It was designed for a minimum of input information and to output according to options. It was further designed such as to allow the response matrix to be input instead of generated under an option control. Its design was such as to make it suitable for future extension to carry out further analysis.

2. DISCUSSION

2.1 THEORETICAL

The detected experimental bremsstrahlung photon number spectrum may be considered as a frequency distribution of monoenergetic gamma photons and the detecting NaI(Tl) crystal as responding to it to produce a spectrum which is essentially a superposition of characteristic monoenergetic spectra. The relative intensity and shape of the monoenergetic spectral components is a function of photon energy and experimental geometry. Their combination in the measured continuous spectrum P over n increments or channels is defined by the system of simultaneous linear equations as follows:

$$\begin{aligned} p_1 &= n'_1 r_{11} + n'_2 r_{12} + \ldots + n'_m r_{1m} \\ p_2 &= n'_1 r_{21} + n'_2 r_{22} + \ldots + n'_m r_{2m} \\ &\vdots \\ p_m &= n'_1 r_{m1} + n'_2 r_{m2} + \ldots + n'_m r_{mm} \end{aligned} \qquad (1)$$

which may be expressed in matrix notation as

$$P = RN' \qquad (2)$$

where

R = system response matrix (m x m)

N' = uncollided photon number flux interacting in the crystal (m x 1)

Mathematically the reduction or unfolding process is accomplished by evaluation of the matrix equation

$$N' = R^{-1} P \tag{3}$$

Since the response matrix only expresses the detector system smearing of detected monoenergetic photons, it is necessary to correct N' to account for the number of incident but undetected photons and so determine N, the incident photon number spectrum; N is given by the relationship[6]

$$N = \eta^{-1} N' \tag{4}$$

where

η = the NaI(Tl) crystal interaction or collision efficiency (a diagonal matrix).

The nonzero elements of η may be determined from the expressions[8]

$$\epsilon = \frac{1}{\Omega} \int_{\text{crystal}} (1 - e^{-\mu x}) \, d\Omega \tag{5}$$

and

$$\eta = \epsilon \cdot K \tag{6}$$

where

μ = the energy dependent total linear attenuation coefficient of NaI(Tl) (It does not include coherent scattering.)

x = the vector path length of a photon in the crystal prior to interaction

Ω = the solid angle subtended at the photon source by the crystal front face

K = a factor to account for photon interactions with the j materials interposed between the source and the crystal.

K is defined by the expression

$$K = \prod_{i=1}^{j} e^{-\mu_i \cdot z_i} \tag{7}$$

In expression (7) μ_i is the total linear attentuation coefficient of the i^{th} interposed material (e.g., crystal cladding) of thickness z_i.

The photon flux number spectrum at the crystal is defined as

$$N_x = \frac{N}{\text{crystal frontal area}} \tag{8}$$

The photon energy spectrum at the crystal for photons of energy E is given by

$$I = N \cdot E \tag{9}$$

and the photon energy flux spectrum at the crystal by

$$I_x = N_x \cdot E \tag{10}$$

The total exposure dose is defined as

$$D = \int_{\text{energy}} N_x \cdot E \cdot \mu_{air}(E) \cdot dE \tag{11}$$

where $\mu_{air}(E)$ is the total energy deposition linear attenuation coefficient of air.

In order to evaluate equation (3), it is first necessary to determine the response matrix R. Although it may be approximated by recourse to the Monte Carlo method,[9] this approach usually furnishes an underestimate since for economic reasons account is not generally taken of the experimental environment effects such as photon scattering from the detector photomultiplier, laboratory walls, detector supports, etc. The alternative and usual approach is to construct the matrix employing the in situ experimental spectra of radioisotope sources emitting one or at most two photon line energies. The vectors of the matrix may then be constructed at required intermediate photon energies by interpolation. The interpolation may be carried out either directly or indirectly by describing the experimental spectra by means of suitable analytic functions of pulse-height and expressing their parameters as a function of photon energy.[6, 10]

The experimental determination of R yields a matrix which when substituted in Equation (3) will correct for the detector Gaussian distribution of pulse-height and the Compton scattering continuum of pulse-heights. The NaI(Tl) crystal iodine K x-ray escape phenomenon is most suitably corrected for by application of Axel's expression for the escape fraction, with respect to the number of photons incident on the crystal,[11] as

$$F(E) \simeq 0.367 \left[1 - f \cdot \log_e \left(\frac{1+f}{f}\right)\right] \qquad (12)$$

where

$$f = \mu_\gamma / \mu_x$$

and

μ_γ = the photoelectric linear attenuation coefficient of NaI(Tl) for photons of energy E

μ_x = the photoelectric linear attenuation coefficient for x-rays of energy = 28.5 keV.

The solution of Equation (3) is best performed iteratively since both P and R are experimental and, hence, approximate and because of likely instabilities in the analytic solutions (oscillations). An a priori knowledge that the elements of N should be zero or positive suggests the iterative method of Scofield which yields elements of N with the same sign as the elements of P, the pulse-height spectrum. Except for this desirable feature there is very little difference between the method of Scofield and the classical iterative method.[12]

2.2 CODE CUBED TECHNICAL DEVELOPMENT

During the present report period--CUBED--a digital computer Code to Unfold Bremsstrahlung Experimental Distributions has been developed in the FORTRAN IV language for the IBM-7094 computer. This code is presently undergoing preliminary debugging and testing prior to proving its logic on sample data.

Code CUBED consists of a main controlling program and thirty-five subprograms. A number of existing subprograms[6] have been availed of, some after incorporation of modifications to enhance their versatility. For the purposes of discussion, the code technical development

is topically subdivided as:

(a) Main and Anciliary Programs

(b) Response Matrix Generation Program, and

(c) Spectral Unfolding Program

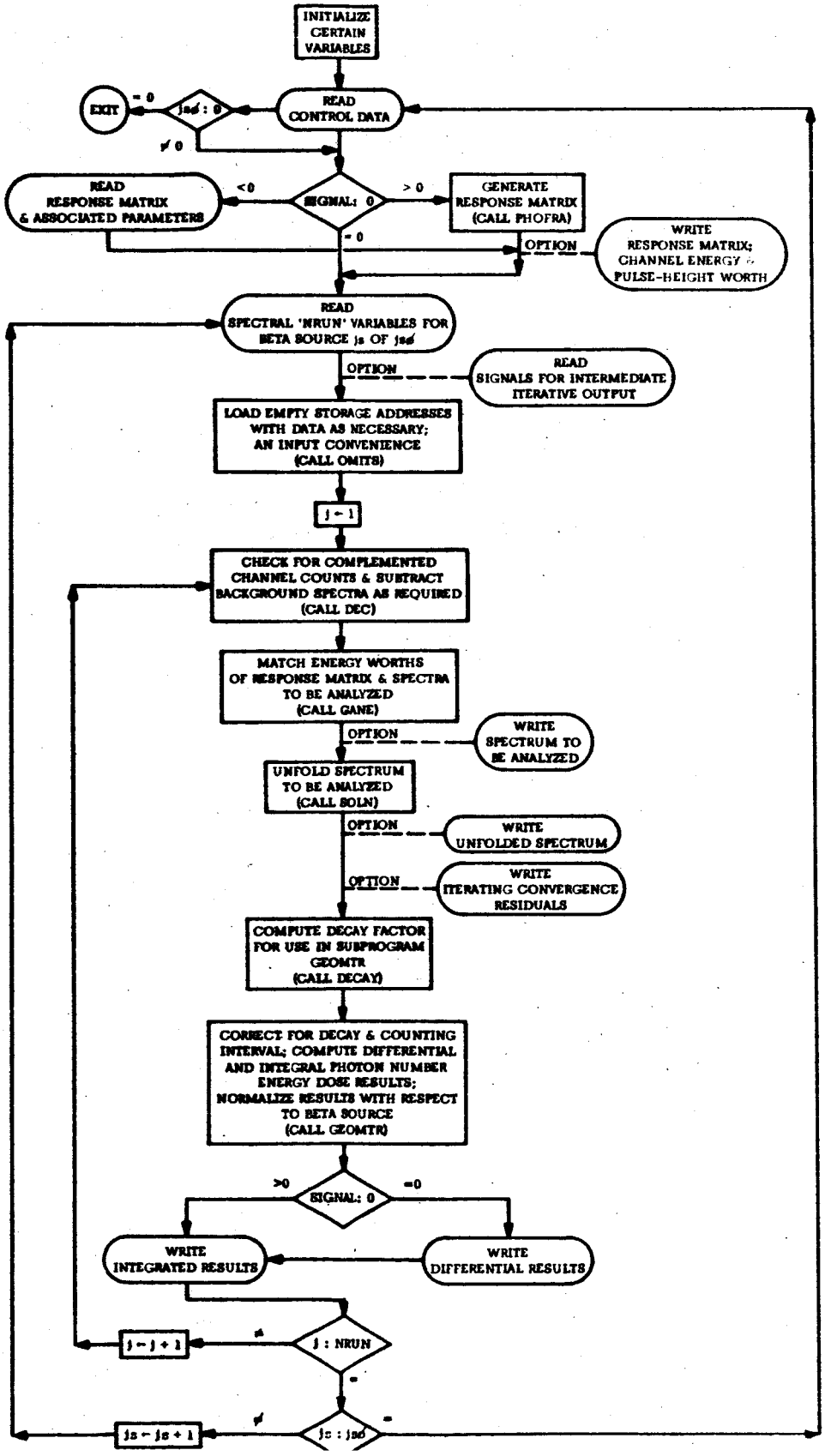
2.2.1 Main and Anciliary Programs

The main program executes data input-output operations, many of them under initially input option signals and provides the major connectivity for the hierarchy of subprograms. Figure I gives a simplified flow diagram of the main program. Details of the input-output variables are omitted from this report since they are still subject to change; for example, it is intended to provide considerable flexibility to the input data with respect to conformity with format statements.

The response matrix generation is carried out under the control of the first subprogram--PHOFRA--called by the main program. Under an option signal it and its associated parameters may be read as a deck of cards instead of generated. The program takes advantage of the fact that data for many of the bremsstrahlung spectra for a given beta source may vary in only one or two variables, and, thus, only these variables need to be input, the unchanging variables being supplied by the calling of subprogram OMITS. Since pulse-height analyzer background subtraction over-subtracted counts are recorded in the complement mode (i.e., as a positive number) these are converted to a true negative number by the calling of subprogram DEC. Subprogram DEC also subtracts a fraction/one/many previously stored background spectra according to option signals. The energy correspondence of the response matrix and the unknown spectra are matched by the called subprogram GANE. The unfolding of unknown spectra is carried out under the control of the called subprogram SOLN, which returns with the photon number spectrum requiring only to be corrected for primary source decay. The decay correction factor is computed by the calling of function subprogram DECAY. Subprogram GEOMTR is called to apply the decay correction factor; to convert results to data per unit time; to compute differential number and energy flux spectra; to compute energy integrated number, energy and dose data; and to normalize these data with respect to both beta source strength and source volume. Subprograms GANE and DECAY are existing programs;[6] subprogram DEC is a modified existing program.[6]

FIGURE 1

FLOW OF MAIN PROGRAM LOGIC. THE CALLED SUBPROGRAMS ARE INDICATED IN PARENTHESES



The main program is designed in such a manner as to make it readily amenable to either extension or subprogram substitution and, thus, suitable for analyzing scintillation spectra originating from other sources than bremsstrahlung such as in, for example, problems of photon scattering.

2.2.2 Response Matrix Generation Program

An evaluation was carried out to ascertain the usefulness of existing available programs for semi-automatically generating response matrices. It was established that a most profitable programming effort lay in deriving an original overall logic especially tailored to the particular experimental circumstances and to use existing programs where routinely applicable. The developed program functions basically as follows:

> The response matrix is generated under the control of subprogram PHOFRA requiring only standard library spectra and a limited number of control parameters as input. The program utilizes a regression analysis routine--STDFIT--to fit photopeaks for subsequent subtraction, to allow the determination of the required Compton continua by interpolation methods in subprogram RESGEN. Subprogram RESGEN interpolates the prior normalized and integrated continua and differentiates the interpolations. After their determination from fitted parameters, the appropriate photopeaks are added to the interpolated continua. The continua are then redistributed, in accord with the nonlinear energy response of the scintillation spectrometer, to construct a normalized response matrix by subprogram PHOFRA. The redistribution employs the existing subprogram GANE, along with other existing subprograms.[6]

The developed response matrix generation program is described in more detail in Appendix 1.

2.2.3 Spectral Unfolding Program

Preliminary research indicated the iterative unfold technique of Scofield to be most suitable for application to continuous scintillation spectral distributions. The unfolding

program is controlled by subprogram SOLN which calls a modified existing program[6]--RESMAT--to execute the Scofield algorithm. Subprogram RESMAT solves equation (3) of this report according to the algorithm

$$N'^{(h+1)} = (D^{-1})^{(h)} P$$

$$N'^{(o)} = P$$

$$P^{(h)} = RN'^{(h)}$$

$$(D^{-1})^{(h)} = \delta_{ij} n'_j{}^{(h)} / P_i^{(h)} = d_{jj}^{-1}$$

where

$$\delta_{ij} = \begin{cases} 1; & i = j \\ 0; & i \neq j \end{cases}$$

and

$$h = \text{iterating index}$$

Iterating is halted when

$$\chi^{(h-1)^2} - \chi^{(h)^2} \leq \text{preassigned value}$$

where

$$\chi^{(h)^2} = \sum_{i=1}^{m} \frac{\Delta_i^{(h)^2}}{P_i^{(h)}}$$

and

$$\Delta^{(h)} = P^{(h)} - P$$

or when a specified number of iterations have been performed. Subprogram RESMAT returns with the crystal interacting photon number spectrum N' as in Equation (3). Subprogram SOLN then calls function

subprogram EFFIC to determine ϵ as in Equation (5), and subprograms AIRABS, PERSPX, and CLAD to determine K as in equation (7). Subprogram SOLN computes the product $\epsilon \cdot K$ to determine η of Equation (6) and, hence, compute N, the corrected photon number spectrum of Equation (4).

Function subprogram EFFIC calls subprogram SIMPSN to carry out the integration of Equation (5), using Simpson's Rule in binary steps according to the relationship

$$\int_a^b f(x)dx \simeq \frac{2}{3}\Delta x \left\{ f(a) + f(b) + 4\sum_{i=1}^{n/2} f\left[a + (2i-1)2\Delta x\right] + 2\sum_{i=1}^{\left\{n/2\right\}-1} f(a + 2i \cdot 2\Delta x) \right\}$$

The function subprogram FC is called by subprogram SIMPSN to determine f(x). Function subprogram EFFIC calls the table searching and interpolating subprograms TA and TE (described in item 1, Appendix 1) to determine the appropriate μ of Equation (5); the energy-dependent μ values are stored in subprogram CO.

Subprogram AIRABS is called by subprogram SOLN to determine the photon interaction factor for air between the photon source and the crystal. This subprogram calls the stored table of μ_{air} values in subprogram AIRTOT. The appropriate μ_{air} value is table searched and interpolated by subprograms TA and TE.

Subprogram PERSPX is called by subprogram SOLN to determine the photon interaction factor for perspex absorbing material interposed between the photon source and the crystal. This subprogram calls the stored table of $\mu_{perspex}$ values stored in subprogram COEF. The appropriate $\mu_{perspex}$ value is table searched and interpolated by subprograms TA and TE.

Subprogram CLAD is called by subprogram SOLN to determine the photon interaction factor for NaI(Tl) crystal cladding material. The crystal cladding material consists of neoprene, polyethylene, sponge rubber and aluminum oxide. This program calls the stored table of cladding transmission factors stored in subprogram ALUM. The appropriate factor is table searched and interpolated by subprogram TA and TE.

3. WORK PROGRAM FOR SECOND QUARTER

The basic code which is presently 85% compiled on the IBM-7094 NASA-GSFC digital computer will be checked for logic faults and then tested on sample spectra. When this testing is complete the code will be applied to typical production spectra. At this point final modifications to the code will be carried out to allow simplification and freedom of input. The desired final format of output will be decided at this stage. The code will then be reviewed from the standpoint of efficiency after which it will be deemed complete.

The work program will be completed after preparation of the code User's Manual has been carried out. This manual will describe the code in detail and contain a theoretical background to code and a sample problem as well as a listing.

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APPENDIX 1

DESCRIPTION OF THE RESPONSE MATRIX GENERATING PROGRAM

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The response matrix generating program consists of a controlling subprogram--PHOFRA--and a lower level hierarchy of subprograms. The proposed logic of these subprograms is described below with reference to the attached figures and to the assigned subprogram names.

1. PHOFRA

The controlling program, PHOFRA, is called by the MAIN program. The main program must supply it with two variables, namely:

N = the matrix size (as in N x N matrix; eg. 20 x 20) and

ELIMIT = the desired energy worth of the upper edge of channel N (eg. 0.40 MeV).

The program design is such that the matrix and the spectra to be analyzed will correspond in energy and pulse-height.

The logic of program PHOFRA is given in Figure 1 of this appendix. It begins execution by calling subprogram DECLIB to read a card deck of standard library spectra. This deck will be as schematically shown in Figure 2 of this appendix. It will consist of NSTAND spectra (eg. NSTAND = 8 for a deck of 8 spectra) of 200 channels; 20 cards per spectrum. Each spectrum will be preceded by one identity card which will contain 5 variables, namely:

ALABEL = the isotopic name of the standard source; eg. HG-203

NSJ = the channel number in the valley below the major photopeak

NFNJ = the channel number of the background above the major photopeak

NSXJ = the channel number of the "flat" below the x-ray peak

NFXJ = the channel number of the "flat" above the x-ray peak.

The last four variables are further defined in Figure 3 of this appendix. The numerical values to be used will be approximations as would be visually read from a pulse-height analyzer display scope. If the particular standard spectrum contains no x-ray peak or second photopeak, the NSXJ = NFXJ = blank. The library deck will be preceded by one card on which are defined NSTAND (eg. = 8) and the number of pulse-height analyzer channels, NPHA, referred to as "dead-channels." (See Figure 3.) In order to analyze the two-photopeak spectra of Na^{22} and Zn^{65}, it is a requirement that the program be supplied with a 0.51 MeV spectrum of a source such as Sr^{85} or F^{18}.

Subprogram SOLIBY is called to identify and order the standard spectra library deck.

Subprogram RESGEN is called to compute NSTAND gain and count normalized standard source continua, as described in Item 4 below. Subprogram PHOFRA then interpolates N normalized continua and adds to each of them their appropriate corresponding Gaussian photopeak and associated K x-ray escape peak. The relationship between photopeak and escape peak is determined by subprogram RAXEL, which table searchs values of the K escape fraction as determined from Equation (7) of this report. The Gaussian photopeak photon energy dependent standard deviation $\sigma(E)$ is computed from an expression of the type[5]

$$\sigma = k \cdot E^n$$

where k and n are determined by a least-squares fit to the photopeaks of the standard spectra in subprogram SVFIT.

As an aid in interpolating, subprogram PHOFRA integrates the normalized standard source continua before interpolation and then differentiates the interpolations. The interpolation is Lagrangian[13], for which subprogram TA has been written; it calls an existing binary table-searching subprogram, TE.[6]

Subprogram PHOFRA next redistributes the N, gain and count normalized, spectra in accord with the pulse-height/energy response of the detector-system, calling subprograms GANE and PULSE to do so. The redistributed spectra are normalized such that their integral equals unity. At this point, subprogram PHOFRA has generated a normalized response matrix of approximately triangular appearance and transmits it to the MAIN program for use as the coefficient matrix in analyzing either

continuous or complex gamma photon spectra measured under the same conditions as the standard spectra.

2. DECLIB

This subprogram reads the standard source spectra; see Item 1 above.

3. SOLIBY

This subprogram identifies and orders the data read by subprogram DECLIB for PHOFRA; see Item 1 above.

4. RESGEN

This subprogram gain and count normalizes the Compton continua of the standard source spectra. It also determines $\sigma(E)$, as discussed in Item 1, by least-squares fitting the NSTAND determined standard deviations of the spectral photopeaks. $\sigma(E)$ is fitted by subprogram SVFIT to determine k and n, called by RESGEN.

In this subprogram the normalized continua are determined by first fitting a Gaussian distribution to the spectral photopeaks and then subtracting the fitted Gaussian. The normalization of the residual, or continuum, consists of a division of the continuum counts by the photopeak Gaussian area, determined in the fitting, and gain changing of the continuum from that gain given by the photopeak pulse-height (from the fitting) to a unit gain of eg. 100 channels. Gain changing is carried out by calling subprogram GANE. Photopeak fitting is carried out by subprogram STDFIT, as described in Item 5 below.

To determine the continua of Na^{22} and Zn^{65} standard spectra, the program subtracts the 0.51 MeV fitted photopeak and its associated continuum. The extent of the associated continuum is determined from the photopeak-to-continuum relationship of an 0.51 MeV spectrum of Sr^{85}; the necessary subtraction is carried out after gain and count matching.

The interfering x-ray peaks in spectra, such as a Hg^{203}, are removed by assuming the continuum to be linear between channel NSXJ and channel NFXJ. This approach has been used previously by workers such as Heath.[10]

5. STDFIT

This subprogram, called by RESGEN, fits a nonlinear analytic expression to experimental data, within the statistical accuracy of the data, according to the Gauss-Newton-Raphson method.[14] The proposed analytic function, computed in the called subprogram FUNUS, consists of a "Gaussian + Cosine-or-Straight Line + Constant." The choice of this function was based on an examination of sample spectra. The fit is carried out from channel NSJ to channel NFNJ. The fitting method and, hence, the subprogram require initial reasonable estimates of the analytic function parameters; these are provided by calling subprogram GUESS.

6. FUNUS

This subprogram is called by subprogram STDFIT to compute the proposed analytic function and its partial derivatives. The function parameters to be determined by the fitting are defined in Figure 3.

7. GUESS

This subprogram is called by subprogram STDFIT to estimate initial values of the parameters required by subprogram FUNUS. The basis for the estimates is a study of typical sample spectra.

8. GANE

This subprogram numerically redistributes, or gain changes, a spectrum.[6]

Other subprograms employed in the response matrix generating program have either been discussed above or are not pertinent to an understanding of the present logic description; they are described briefly as follows:

GAUSS[6]: computes a Gaussian photopeak of given area, standard deviation and pulse-height; called by subprogram RESGEN.

PEAKS: adds photopeak and escape peak to Compton continuum and normalizes sum with respect to spectral area; called by subprogram PHOFRA.

SC:	tabulated K x-ray escape fractions.
ENERGY:	tabulated deviations of pulse-height from linear response.
RAXEL[6]:	control for subprogram SC.
PULSE[6]:	control for subprogram ENERGY.

FIGURES

NOTES:
1. R = K X-ray escape fraction
2. δV = fractional deviation of pulse-height from linear response

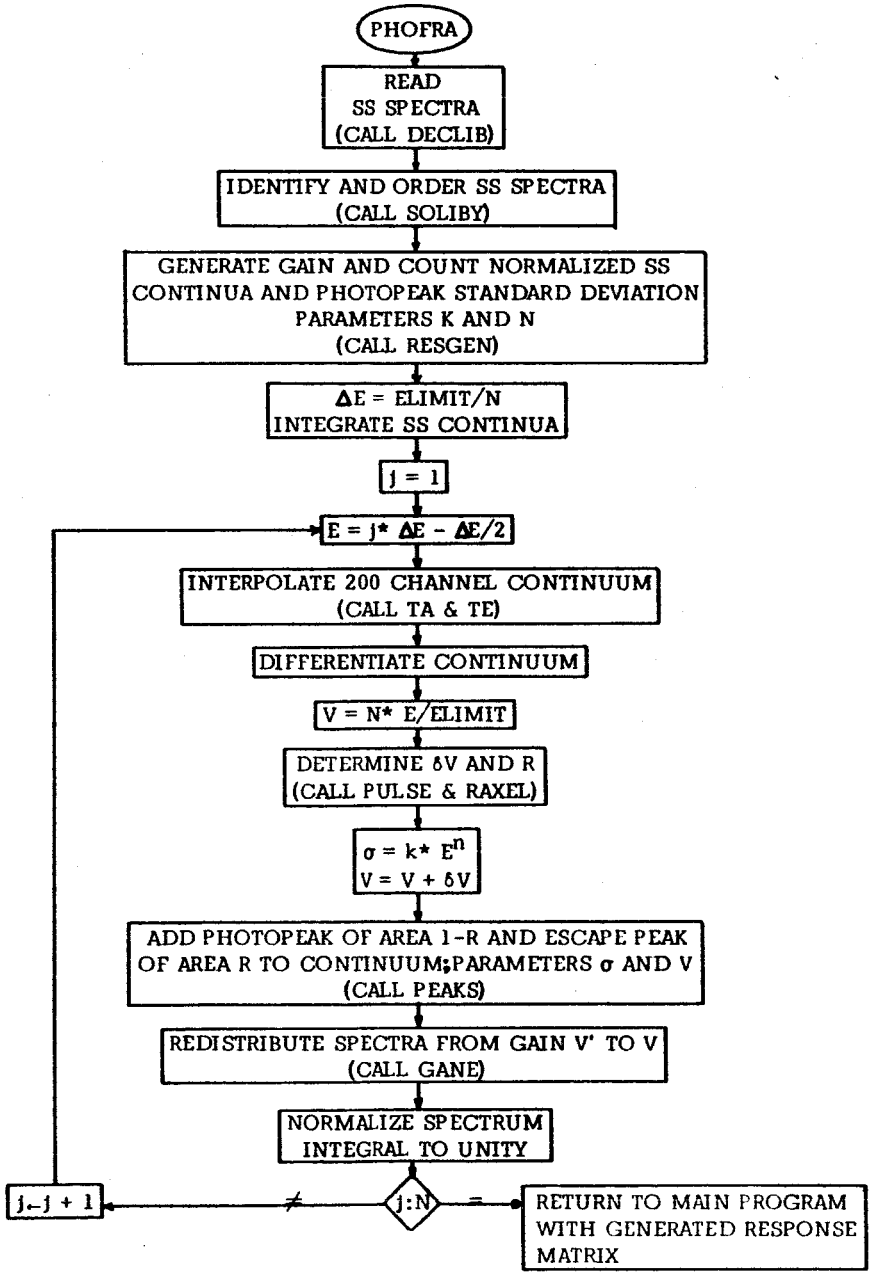
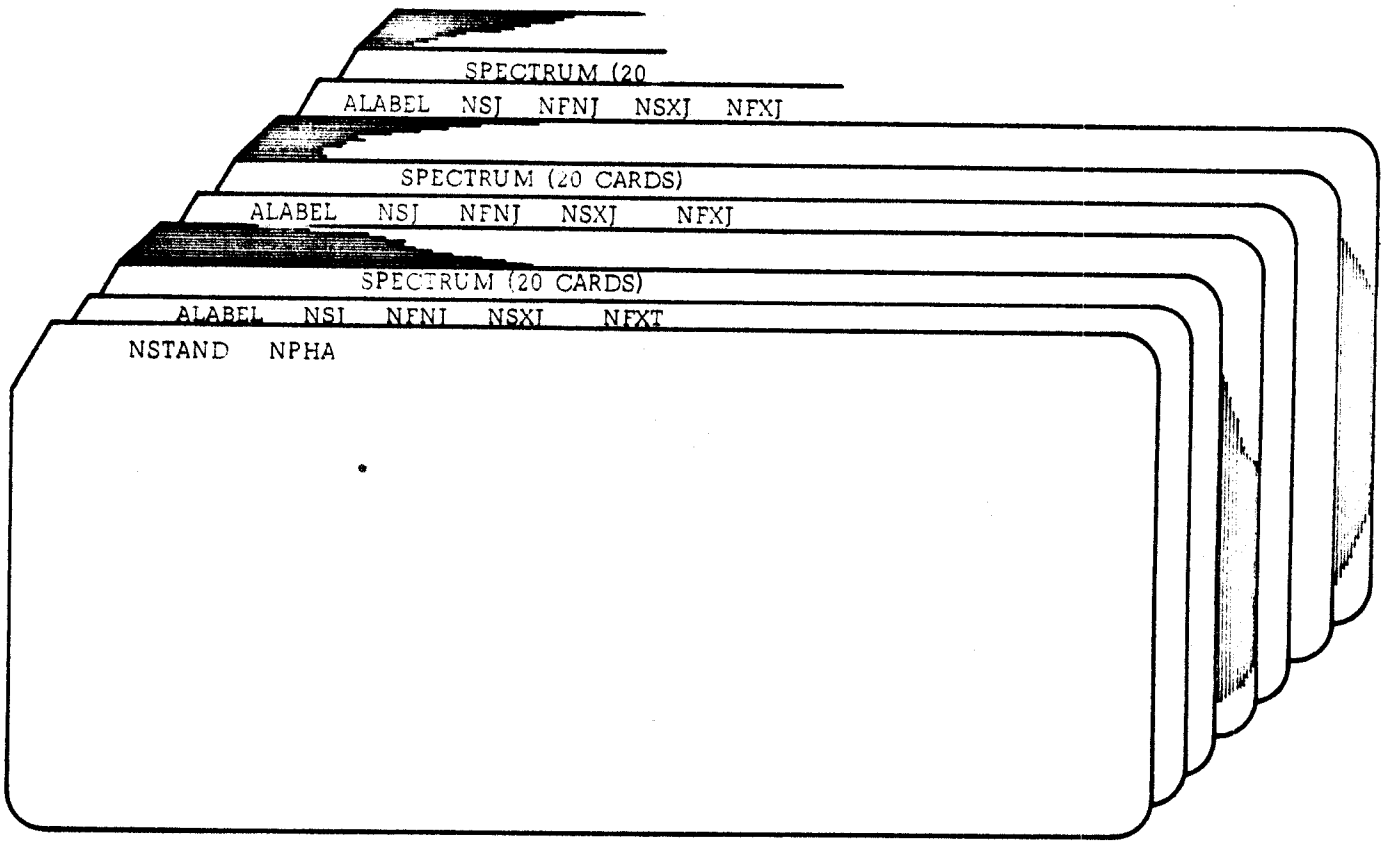
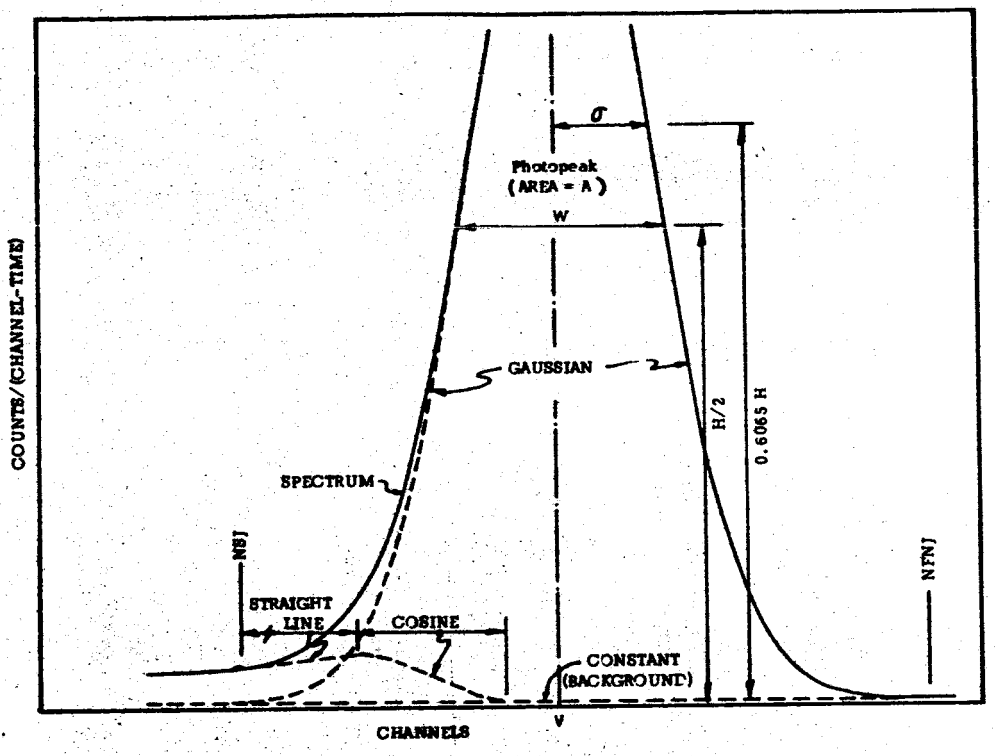


FIG. 1

FLOW DIAGRAM OF RESPONSE MATRIX GENERATING PROGRAM LOGIC;
SUBPROGRAM PHOFRA.

FIG. 2
STANDARD SOURCE SPECTRA LIBRARY DECK ARRANGEMENT





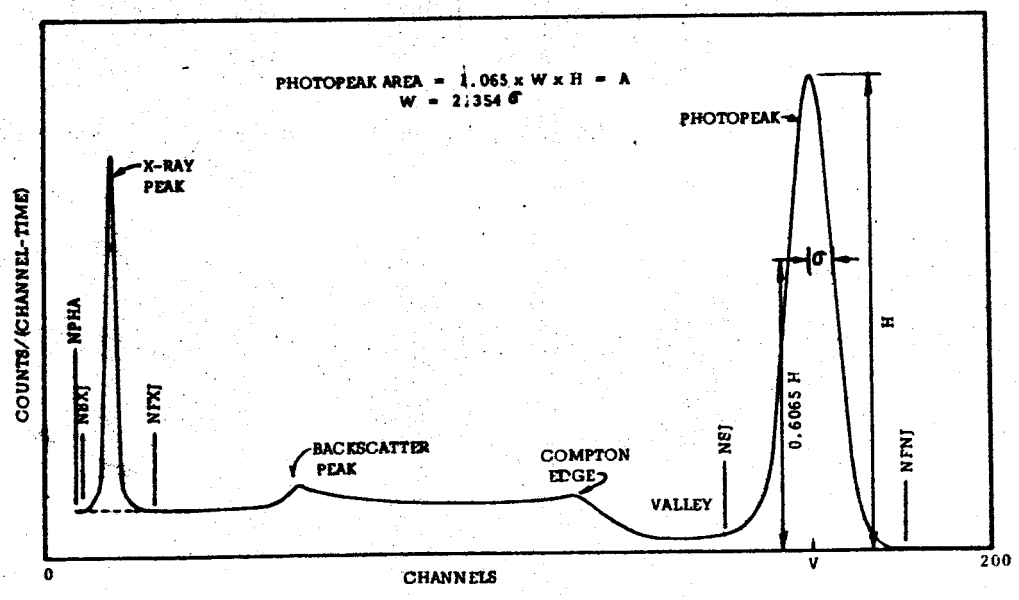


FIGURE 3
FIGURES DEFINING SPECTRAL VARIABLES FOR SUBPROGRAM RESGEN