PRNC160

PRNC. 160

PUERTO RICO NUCLEAR CENTER

COMPUTER AIDED DECOMPOSITION OF GAMMA SPECTRA

EMITTED BY CERTAIN RADIOACTIVE NUCLIDES

By

Aviva E. Gileadi and Nallagounder Kuppusamy

OPERATED BY UNIVERSITY OF PUERTO RICO UNDER CONTRACT

NO AT (40=1=1833 FOR US ATOMIC ENERGY COMMISSION

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ersity of Puerto Rico

Mayaguez Campus

COMPUTER AIDED DECOMPOSITION OF GAMMA SPECTRA

EMITTED BY MIXTURES OF CERTAIN RADIOACTIVE NUCLIDES

by

Nallagounder Kuppusany

A thesis submitted in

partial fulfillment of the

requirements for the degree of

Master of Science

(Qluclear Engineering)

January 1973,

Approved:

af a Wa leeed Rey 1692

airman Graduate Committee a

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ABSTRACT

A computer code PRGA, written in FORTRAN IV, has been developed in order to perform decomposition of certain ganma spectra obtained by means of Ge(Li) diode equipped multichannel data acquisition system. The code uses spectra of the individual standards and those of the mixtures as input data and calculates the mixing factors pertinent to each component, using Linear least squares fit techniques.

PRGA is presently operative on both the IBM-360/40 and the PDP-DEC-10 computers at the Computer Center of the University of Puerto Rico, Mayaguez Campus. The code includes

corrections designed to account for deadtine losses, natural

and spectral background, decay and counting statistics. Using source mixtures with premeasured mixing factors, specially prepared for the purpose of comparisons, it was found that the premeasured and PRCA computed mixing factors are in satisfactory agreement.

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It is the authors wish to express his gratitude and sincere thanks to those who helped him to complete this project:

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component source mixtures. Compgnents: 11Na??,

Freoeo, 2ohnee, Deine and SoeotsT 7

A,1 Avpangenent of input card deck for PRGA-Code. 6s

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CHAPTER I

INTRODUCTION

During the last decade or so the development of 1ithium

érifted germanium detectors requiring cryogenic techniques and associated low noise electronics and the use of such de~ tectors with various sophisticated data acquisition systens, featuring such itens as multichannel analysers with large memories, often interfaced with digital data processors - made 4 considerable impact on experimental photon spectro- retry.

Inprovenent of the experimental techniques resulted not only in higher accuracy, and better resolution, but also in an unprecedentedly large quantity of available gamma spectral @ata. In order to match the efficiency of data acquisition Yo that of converting these data into meaningful information: numerical techniques are required.

Such techniques not only provide considerable savings in time but also significantly improve the accuracy of data a- nalysis.

Ideally even the most complex spectra should be analys- able, qualitatively as well as quantitatively, with little or no man-nachine interference. However, before such rather ambitious objective could be achieved, several simpler par- tial programs need to be developed and checked out, each of

?them designed to perform a partial task in the framework of

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complete analysis. Once all the partial programs are opera~
tive, they are integrated into a complete system, capable to
determine background, to resolve and fit complex peakgroupings,
to determine the energies and intensities of the gamma rays
a9 well as the amount of source nuclides within the analysed
mixture.

?The Nuclear Engineering Departnent of the University of

Puerto

ico, recently acquired a high resolution gamma detec-
ting system consisting of a lithium drifted germanium detec-
tor, (manufactured by Princeton Gamma-Tech) to be used in
conjunction with a multichannel analyser (model No. 88-015
manufactured by Nuclear Data, Inc.). This system is to be
used in a rather extensive neutron activation project planned
by the Department.

Tt is felt that a reliable and efficient computer code-

written especially for analysing data,acquired by the above described, Ge(Li) diode equipped,gamma spectrometer would be a welcome contribution to the departamental efforte in the field of neutron activation.

With this general objective in mind, and as a first step towards it - in the present thesis a computer code PRGA was developed that is capable to decompose gamma spectra emitted by certain source mixtures

PRGA is written in FORTRAN IV and is operative on the IBN-360/40 Computer at the University of Puerto Rico, Mayaguez Campus Computing Center. The code has been tested

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on gamma spectra en!

?ted by several different preneasured source mixtures and its performance has been found satis~factory.

#11 gamma spectra used in testing the PRGA code were acquired by means of the Ge(Li) diode equipped gamma ray detector system of the Radioecology Division of the Puerto Rico Nuclear Center, the deseription of which is given in

Chapter v.

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CHAPTER

REVIEW OF LITERATURE

Ganna ray spectronetry is anong the most versatile, most important ané most frequently applied methods of modern science, accordingly, the professional literature pertinent to that subject cannot be exhaustively reviewed within the scope of the present thesis. An attempt is made, however, to briefly review a selected set of outstanding original papers on the subject of computerized decomposition techniques (Yunscrambling") of gamma spectra.

J. MILLS (1) has developed a computer program AUTSPAN for analysis of complex gamna spectra obtained with Ge(Li)

detectors. The program contains options for data smoothing, peak location and determination of peak parameters.

G. D, ATKINSON Jp., J. B. WHITWORTH and S. J. GAGE (2) have written a code, NAA, which seeks out peaks, locates the peak maxima, predicts Compton knees, single and double escape peaks and identifies the unknown nuclides present. The code is written in FORTRAN TV and operative on the coC-6600 computer.

JEAN KERN (3) after a review of the most accurately known gamma calibration lines, presented a method of obtaining new secondary standards of sinilar precision, but ex-?tending to higher energies. Her method uses simultaneously

pair peak method, energy combinations and experimental non-

---Page Break---

Linearity curves.

W. C. WHITE, M. B, SHAPTRO and A. W. PRATT (4) applied Linear progranning to deconposing spectra.

J.T, ROUTTT and S. 6. PRUSSIN ($) have written a For

?tran program which searches and fits the cingle and multiple peaks. In addition their code performs the energy, efficiency, Line shape calibration, and error estimates.

The program given by R. GC, HELMER, R. L. HEATH, M. PUTNAM and D. Hl, GIPSON (6) computed the gamma ray energies and intensities and provided an estinate of uncertainty, by fitting the gamma ray peaks to a Gaussian and applying a correction for the nonlinearity of the electronic syetem,for the data obtained both by NaI(T1) and Ge(Li) detector systems.

R. GUNWINK and J.B, NIDAY (7) have constructed an elaborate program, GAMANAL, which determines the background, ?the energies and intensities of the gamma spectrum and the amounts of the source nuclides present in the mixture.

Taking selected channels of data of puleeheight distribution F. D, KNIGHT (8) applied the method of simultaneous linear equations to find the abundance of the concerned nuclides present with the knowledge of the component spectra and the composite spectrum.

The computer progran, CAUSS-V, developed by R. @. HELMER

and M.

PUTNAM (9) locates the gamma ray peaks, determines the peak parameters, finds the gamma ray intensities and energies applying nonlinear least square curve fit for the

---Page Break---

pulse height distribution obtained with a Ge(Li) detector system.

M. CIAMBI, L. DADDI and V. D. ANGELO (10) have fitted the ganna ray photo peaks to a Gaussian, using a maximum probability method and compared the results with those obtained by the least square method.

W. W. BLACK (11) used conrelation techniques to locate the photo peaks, he analysed pulse height distributions obtained with Ge(Li), Si(Lid, and MaI(T2) detectors. Ile also applied thie method to data obtained by means of neutron tine of flight analysers.

An early paper of J. H. HUBBELL and N. E. SCOFIELD (22) deals with ?unscranbling" experimental ganna spectra using

matrix techniques.

WALTER F. BURRUS (13) used Fourier techniques to obtain the ?unscranblea" spectrum an¢ has assigned meaningful error-estimates to the results.

a

WEST Jr. and 8. JOHNSON (24) discussed an un-folding code for the IBM 650. They described a procedure for removing scale and energy dependency.

R. L, HEATH, R. G. HELMER, L. A. SCHMITTROTH and 6. A.

CAZTER (15) used interpolation betueen experimental spectra, to calculate pulse height distributions obtained by NaI(T1)

crystal system for sources emitting only one gamma ray.

GEMRKE, J. E. CLINE and R. L. HEATH (16) developed

e method to determine both the relative detection

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efficiency and the Linearity of the Ge(Li) detector system.

+ G. HELMER, R. G, GREENWOOD and R. J. GEHRKE (27) have measured the energies of ganna ray photons from 24 nuclides using a Ge(Li) detector and have applied correction for the nonlinearity of the detector syste and for the recoiling nucleus.

MARTE PUTNAM, D. H. GIPSON, R. G. HELMER and Re L. HEATH (18) developed @ computer program which performs a nonlinear least squares fit to pulseheight distributions, obtained both fron NaI(T1) end Ge(Li) detector systens. Their program fits the data to their modified Gaussian functions and prints out the peak paraneters.

The program described by R. L. HEATH, R. G. HELMER, L. A. SCHMITTROTH and G. A, CAZIER (19) snoothens the gamma ray spectra, applies correction to the gainshift of the detector

system and fits the data Gaussians using linear least squares criterion.

H. BABA, H. OKASHITA, S. BABA, T. SUZUKI, Hl. UMEZAWA and Hi. NATSUME (20) constructed a program to analyse ganma Pay spectra obtained by using a Ge(Li) detector. The analysis is based on the first derivative method associated with a number of peak shape tests. The effects of data smoothing and change in peak width were studied.

K. LOW (71) attempted to find the contribution from known nuclides in a complex gamma ray spectrum, using least

squares method.

---Page Break---

FILIPPONE and F. J. MUNNO (22) discussed the influfence of deadtine losses on the magnitude and shape of the composite spectrum obtained by means of a multichanne? ana~lyser, They presented a relation including appropriate corrections.

R. G. WAGGENER, L. F. ROGERS and P. ZANCA (23) Health Physies published @ matrix method to correct for non Linear energy response of NaI(T1) spectrometer systems.

R. K. GILLETTE (24) has developed @ computer program for the analysis of neutron activation data containing an option for smoothing gamma spectra.

J. I. TROMBKA (25) developed a least squares fitting technique for the analysis of complex gamma ray pulseheight spectra, synthesizing the polyenergetic distribution from a series of nonoenergetic components in the incident bean.

H. P. YULE (26) published an exhaustive review paper fon computation of experimental results in activation analysis.

D. D, TUNNICLIFY and G. E. A. WYLD (27) have developed 4 code, based on linear least squares, that computes directly

?the weights of the components in a source mixture.

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CHAPTER T1T

THEORETICAL BACKGROUND

In the literature numerous methods have been described, for computer aided analysis of gamma ray spectra obtained with Ge(Li) or NaI(T1) detector-cystems. In most of these methods the analysis is performed with the aid of calculated or measured response functions corresponding to moncenergetic photons or individual isotopic components of the sample.

?The physical and statistical phenomena determining the response of a semiconductor type detector to a moncenergetic gama photon, incident on it, are quite complex and the accurate fundamental calculation of peak shapes for the purpose of spectrum analysis is quite difficult. For this reason and because the peak shape may be sensitive to small variations in experimental parameters, it ic desirable to determine a mathematical representation of the composite spectra directly from meacured data.

In order to assign a suitable functional representation, it is important to examine some of the factors that determine the peak shape. The primary factor determining the width of a photo peak is the statistical fluctuation in the division of the observed energy between sonization and heating of the crystal lattice. This gives rise to a Gaussian distribution

is die-

1th. The extent to which

with a small specified u

trivution is reflected upon the experimental data, taken with

---Page Break---

a particular system,ie dependent on a number of factors. The material properties and the impurities in the detector affect the charge collection and the electronic noise associated with the leakage current.

The combined effect of incomplete compensation of impurities and incomplete charge collection worsen the resolution

and give rise to low energy tailing of the photo peak. At

low energies the contribution to the resolution from preamplifier noise is important and at higher energies the inabilities of the amplifier and the pulscheight analyser begin to affect the line width, especially when long counting ?mes are involved. Although the use of the digital gain stabilizer can decrease the broadening, the stabilization may itself change the shape of the peak.

Finally random summing of pulses at

gh counting nates
broadens the peaks and gives rise to tailing. The continuum under the peaks is due to Compton distribution from higher energy ganna rays and general counting background. Without detailed knowledge of the composition of the spectrum we can only say that the continuum in the short interval under one peak on a cluster of peaks is, except for statictical fluctuations, a continuous smoothly varying function of energy. Such a function can be approximated with « polynominal.

Anong the several techniques used in computer aided

Gecomposition of complex gamma spectra three major ones will

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na

be discussed briefly, following references § and lit

(a) Linear least squares technique

(b) Non Linear least squares technique

(c) Correlation technique

In the linear least squares technique the pulse height spectrum due to a polysnergetic distribution of ganas rays is eynthesized by using 2 series of normalized pulse height distributions, due to either ronoenergetic components or to the pulse height distribution characteristic of various sin-gle mictides in the source-mixture. Each of these pulse height distributions is weighted so that their sum is a best fit based upon a least squares criterion to the experimentally cetermined polyenergetic pulse height distribution due to the Source mixture under consideration.

It is assumed that the data points in a portion of the

experimental spectrum can be represented by a function

wnich depends on a set of paraneters p,. The purpose of a

least squares fit is to find the value of the parameters,

which minimizes the sum of the squares of the deviations of

the data from the function; that is

De fen]? an

is minimized. The 9,0 are experimental data points, the wy

are the weights associated with the y;, and the 9; (p,) are

---Page Break---

the values calculated from the function used to represent the data. The summation is overall the data points used in the fit.

A necessary condition for R? to be a minimum, as a function of the py, is that the set of equations

ar?
? o for k = 1,2,
Pj,

(3.2)

hold simultaneously for all values of k.

If J, is a Linear function of the parameters p,, the problem is a linear least squares problem, and expressions can be derived for the "best" value of the parameters. However, if the function is not linear in the parameters, no explicit solution of the equations exist. In this case a ne-

thod of "Linearization" may be used.

One such method of Linearization is that of Cause. Thi method consists of Linearizing the function with respect to @ set of parameters 4p, by the use of a truncated Taylor series. Initial estinates, pf, of the parameters must be available in onder to evaluate the derivatives in the expression; that is:

on Fee) = 362) oH

Pe FPL BP and FPR) = HEH9) dim t

---Page Break---

plus expressions containing higher derivatives, where the Gerivatives are evaluated at the initial values of the paraneter.

Te function 9(p,) is a Linear function of the p, if

all derivatives beyond the first are neglected. This gives

2

Rn? = Sw [yy - 699) - SAY 3.3)

> af: Hen sp Pk

The conditions which now determine the minimum are given by

aR/8C 3%) = 0 fork = 1,2, 0.8 (3.4)

this gives as many equations as there are paraneters pj.

?The solution of this set of equations can be represented

in a compact form by the use of matrix notation. Let the de-

sired changes in the parameters be given by the vector

ap = COP)s BPys bPy as)

Let the vector B be defined as:

5 [Dao = P09

0; ~ IPC BIz/ apydene

8)

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Ww

The cosfiicients of the gp, are vepresented by a synme-

tric matrix with the elenents

cn

The set of equations can now be written

caps p Where AP and P are column vectors.

The solution is AP = A.8, where the matrix a = c7},

Since the higher devivatives have been negiected in e-
quation (2.3)this process does not yield the solution of e-
quation(3.2). Therefore, equation(3.u}se solved agein with
the af replaced by (oP + spy). This process is repeated in
an Sterative sanner untél all the jp, ane less than sone
such that the iterations stop if py ? ay for all i si-
multaneously. At this point the fitting process is con-
cluded for enis peak.

Th order to apply the non linear least squares m

hod
to pulse height distributions obtained by means of a Ge(Li)
detector system, the following should be considered: A ge-
mma ray spectrun,obtained with a Ge(Li) detector,coupled to
@ multichannel analyser,consists primarily of a emooth con-
?nuous distribution on which is superimposed @ series of

Peaks. et a portion of this spectrum be represented by

---Page Break---
as

5+ Dy ty ro)

7

here

¥55 vo3ie*[1 # LGR + 2250; 5)?] G3)

with

Gay

is a line which represents the continuous distributions

In a complex peak the subscript j identifies the Gaussian

in equation (3.9); the powers m, and m, are predetermined,

2

even positive integers. The Gaussian paraneters x, (center

of photo peak in channels), yo (count at peak or x,).¥, (full

width of peak at half maximum in channels) can be determined

in the fit. The parameters «, and «,, which represent the

2 "2

deviation of the photo peak from a Gaussian, can also be de-

termined, The line parameters a (value at first channel in

fit) and b (slope) can be determined in the fit. In some

---Page Break---

1s

cases the a, and a) terms have been used in fitting photo

peaks from NaI(T1) data, but a Gaussian function i.e.

zo a2)

The correlation technique utilizes the cross correlation

"

c(r)=Lim 51 ff (terddt when T?» co 3.13:

afew :

:

distribution of the complex spectrum). Assuming that

a(t) = af (ten as)

where a is a constant and n represents random noise and ap-

proximating f(t) and g(t) with a set of diserete values, the

cress correlation function can be approximated as

ce > f begs cas)

where t andr are integers (e.g. channel numbers). or the

purpose of discussion f(t) is referred to as search spectrum,

---Page Break---

a

a(t) the data spectrum and C, as the corre! spectrun.

According to its definition, the cross correlation function is generated by forming the products of £, , and g, keeping the search function sliding by one unit to the left each tine ?ie increnented by one. Thus C, will have a peak, whenever the peak in the search spectrum overlaps itself in the data spectrum, This fact can be used to localize monoenergetic components in the polyenergetic spectrum. In order to do so successfully, it is necessary to find a method of enhancing the structure in the correlation spectrum; it is also desirable to remove all of the background not associated with the structure, Assuming that the data structure has a form

of

=f . G18)

with b constant it can be seen that

flay, D0 if teem

and Gan

fee, to ar term

where M is the number of points in the search spectrum f(t).

?This accomplishes both requirements, enhancement of

the structure and supression of background. Therefore the

expression of C, may be modified to read:

---Page Break---

le

c+ Bete]

A, = Ss,

when applying this method to actual data, certain mod-

ifications have to be introduced in order to take care on

random fluctuations. It is clear that the term

Seer

will no longer vanish beyond the structure for data where A

is fluctuating in a statictical manner, However, renenbering that the computation of A, , as given by equation (2.18), it can certainly be expected that fluctuations of one standard deviation or more would be smoothed out. Therefore the square root of A should be sufficient to suppress statistical fluctuations. With this in mind, the modified equation for C now reads:

ce Ds: [ewe ve] @as

When applying the cross correlation method to decomposi-

tion of pulse height spectra, the search spectrum is a Gau-

| (3.20)

ssian, therefore

Ylewras ove

---Page Break---

where

pam = abyint Qa

The only input parameters are the window width # and the

Fut, Ng is @ constant.

Figures 3.1 and 3.2 contain the pulse height distributions

(ata spectrum) and the pertinent cross correlation functions

obtained using appropriate search spectra, plotted on the same

@iagran. Figure (3.1) refers to a spectrum obtained by a Ge(Li)

detector. Figure (3.2) to one obtained by a NaI(T1) crystal.

Both figures (quoted from reference 11) illustrate the

effectiveness of the cross correlation method in locating

peaks.

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(ut 92us49j94 oss)

ze 3unoTd

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CHAPTER Iv

MATHEMATICAL BASIS OF THE PRGA-CODE

?The PRCA code is based on a mathematical mode) using Linear least squares techniques to calculate the mixing factors of a multicomponent spectrum.

In its simplest form, the problem may be formulated in

the following manner:

Given the pulse height distribution spectrum of a source mixture, obtained by means of a certain gamma ray detector system, as well as normalized pulse height distribution spectra of the individual components obtained by means of the same ganna ray detector system, the mixing factors are to

be determined,

In order to obtain @ numerical solution of thie pro-

Diem, the following mathematical model is used:

Let S(I,K) denote the count rate in the K th channet

due to the I th isotope

C(I) the T th mixing factor to be determine

TK) the count rate in the K th channel due to

mixture (given)

TL the total nunber of isotopes used in the

mixture (given)

KK the total number of channel used (given)

Under the assumption that T(K) the count rate in the

---Page Break---

K th channel due to the source mixture is produced by a linear

combination of count rates corresponding to each component,

TCX) may be expressed as:

700 > C(1)aS(15K)

Tal

. kK aay

In order to determine the optimal values of the C(I)

mixing factors a linear least squares fit is used, searching

for a minimum of the function:

KK

i

5 2

D Do freo-|Eecrescevof] 29

i

<r

Uys oye

with respect of the choice of the C(I) mixing factors. The

minimizing C(I) values are determined by differentiating U

with respect to each C(I) and setting the derivatives to

zero. This leads to the system of linear equations of the

Following form:

a Lh

leading to

zp

Sreosses.0 DLew [Lecco]

Tr Kel

a)

for J =1, 2, ...1T cs)

---Page Break---

denoting

and

KK

Bevorea.w = ac.07 wn

A

u

Sacsecey = ae we)

TA for Je1,2, 6.12

The solution of the set of this systen of equations

one obtains

yields the desired C(I) values.

To execute the above computation of the C(z) values,

@ computer progran PRGA was developed. The arrangement of

the card deck and the listing of the program are presented

in APPENDIX I.

PRGA is written in FORTRAN IV, level 19, and is operative

fon the IBM 360/40 and on the DEC-PDP-10, both at the University

ef Puerto Rico, Mayaguez Campus, Computer Center.

In order to facilitate the debugging procedure, the PRGA

vet tested on a simulated problem, which assuned a source

ixture consisting of ten components and data from forty one

channels.

After its performance on the simulated problem has been

found excellent, PRGA was applied to actual experimental data,

an? the computed results found to be in satisfactory agreement

with premeasured control data.

---Page Break---

A brief description of the experinental equipment and Procedures as well as a detailed comparison of the experimental mixing factors with those computed by the PRGA progran are given in Chapters V and VI.

The performance of the PRGA has been improved by the inclusion of several routines for various corrections, The mathenatical basis of these routines is briefly presented below:

a. Dead time correction was taken into account by first including the system dead time ae an input parameter then correcting each raw count rate reading

8 in the following wa;

8 (4.9)

ms

where S is the raw count rate per second and is

?the system dead time in seconds. Dead time values

used in this paper were computed from the percent

values automatically recorded by the counting sys-

tem. No attempt was made to include channel and

half Life dependent dead time correction such as

advocated by W. FILIPPONE and F. J. MUNNO (see

ref. 22) in the code,at this stage of its develop-

ment, primarily because all control data referred

to sources with half lives of several tens of days,

thus the advocated correction would be negligible.

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Correction for natural background ia made simply by

including the appropriate background count rates

BB(K) as inputs in the program and by replacing

S(ILK) S(T, K)-BB(K) (4.20)

for K = 2,2) 04. KK

Corrections related to counting statistics. Due
the inherently random nature of radio active dis-
integration, allowance had to be made for the sta~
tistical fluctuations in the count rates. This
vas accomplished by assigning a weight factor w,

e

to each value of

u

fra « Secrsosce

modifying the function entering the least squares

fit in the following manner:

«Yh [ro- Frcoren]? wan

é

Cgrrection for Conpton scattering was made in a

purely heuristic fashion,by deducting the pertinent

ordinates of an appropriately chosen linear function

from the measured values. Ascuming that the peak

occurs at

fo and the tangential points $ at K\-M

---Page Break---

near function to be deducted is

resp. K,# the

given by

vei + EEO ysraay (wae)

and the proper correction consists in replacing

SCO =? 8(7,10-¥CK) for

KS KM, KML, cess Kottt easy

Admittedly, the nonlinear method of fitting the in-
@ividual peaks to the sum of a Gaussian and a linear
funetion, as described in Chapter III, is better jus
tified from the theoretical point of views it should
be observed, however, that even the above described
simple Linear routine is ueed by several authors

(refs. 5, 9) and that ite use in PRGA yielded

satisfactory results.

Decay corrections are necessary when the code is
applied in neutron activation analysis involving
short Lived isotopes.

In order to understand how this correction has been
applied let us consider the time behaviour of a single
isotope's activity assuming that

0 to ty - is the irradiation tine

ty to t, - is the cooling tine

ty to ty - is the counting interval

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ALG)

28

the activating flux

is the decay constant of the i-th isotope

is the activation (microscopic) cross

section of the nuclide producing the i-th

isotope

the tine dependent activity of the i-th

isotope

the tine dependent number density of the

i-th isotope and

the number density of the nuclide, the

activation of which yields the i-th isotope.

Under these assumptions the following holds:

Be dow agnpcer octet, ww

=

leading to

Neo = Mgef. ost] o<tety was)

during cooling, i.e. when ty< t<ty

uted = BOeifie? Mt] fen Aneta] (w.a6

and during counting, i.e, when tye t<ty

goo +» MBs e sale

dco] a7)

---Page Break---

The activity of the sample at any instant of the counting

interval is given by: t, t ty

Ay CDE AN, (E)=NS a, (1-e?Nita eo? (tty) (wae)

Therefore the count rate due to the i-th isotope will be pro-

portional to: os

S

va Wait, | ast

[sonaviiefer? joe ee =

, a ws)

Peo b- 4] fewert oer]

Hence in the case of a mixture consisting of short lived isotopes the mixing factors that will result from the least squares fit - described above - will depend upon ty, ty,

tae ez» and ® and in onder to get mixing factore characterizing the composition before irradiation, the following correction has to be applied:

cect

(4.20)

---Page Break---

Fron the mixing factors, CC(I), of the unirradiated
sample, the actual weights are computed by using the nor
nalized activities ané weights of the corresponding standard
samples.

In order to compute the weights of the individual com
ponents in the unirradiated mixture, the following basic

equation has to be used:

es mrittct) -aitets] [ayy

= re

20 = @D Hara accare |

oL %

ap

wnere:

100 = observed counts in channel K

© = neutronfiux

WO) = weight of the J-th isotope in the sample

AGG) = specific activity for radioisotope J at

channel K

i decay factor for radio isotope J.

The validity of the above equation is subject to the

following restrictions:

(a) The number of counts observed for any component

is directly proportional to the amount of the com-

ponent present.

(>) The spectra is additive.

(©) The flux remains constant during irradiation.

(2) The"deadtine" of the data acquisition cysten does

not change during any counting period.

---Page Break---

?This results in a set of equations equal in number to
the nunber of channels. If the specific activities A(x,s)
have been determined by prior calibration, the this set of
equations can be solved for the unknown weights WO) using

least square techniques.

a1

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CHAPTER V

EXPERIMENTAL PROCEDURES AND EQUIPMENT

The performance of the PRCA code was evaluated by com-
Paring premeasured mixing factors with those computed by the
code.

Standard sources and source mixtures were prepared from
4 set of liquid reference sources manufactured by Atomic De-

velopment Corp.. The set included the following nuclides:

wucLIDE | MOST PROBABLE ENERCTES | HALF LITE

Mev

Na?2 0.511, 1.275 2.82 yr.

nn 0.829 200 days

co?? 0.122, 0.136 270 days

co® 2.273, 1.392 5.2 yr.

cs?87 0.662 30 yr.

In order to ensure adequate accuracy self filling lambda

Pipettes were used for measuring radioactive liquies.

Health Physics regulations and instructions referrin

z to

handling open sources were strictly observed. After receiving

the reference sources, they were tested for leakage by the

---Page Break---

PRNC - Health Paysics Division (see copy of leak test report).

All operations involving liquid sources were performed under

a hood, with the experimenter wearing protective gloves.

Standards and mixtures were prepared at the same tine in order to avoid errors due to decay. An aliquot of the reference liquid (e.g. S004) was pipetted on a planchet. A multiple of that aliquot was entered into the planchet that was designated to hold the mixture. Care was taken to deposit the liquid at the center of the planchet in order to preserve identical geometry as mich as possible. All sources were dried under a lamp and after drying all were covered with thin plastic covers.

Al sources were counted on the Ge(Li) spectrometer of ?the PRNC Radioecology Division.

A block diagram of the counting equipment is shown in Figure §.1 and a list of the components is given below.

Ge(Li) detector and associated data acquisition systen

components:

Hv ~ High voltage power supply, manufactured by Hewlett-Packard; model No. 3015.

GecLiy - Lithium drifted germanium detector, manufactured by Canberra Industries Co.;

model No. 7229-240; with cryostat model

No. 7500.

PRE AMP Preamplifier, manufactured by Canberra

---Page Break---

G3LVIDOSSV ONY YO1931.30 (17) 29 40 WYYOVIO 49078

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Us auno1g

W3LSAS NOILISINODY viva

aM

vow

20v

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fuauiam3aAs

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Industries Co.; model Wo. 979,

AMP - Main Amplifier, manufactured by Tennelec;
model No. 70200.

abe ~ Analog to digital converter manufactured
by Hewlett-Packard, model No. 160.

Mea ~ Multichannel Analyzer, manufactured by
Hewlett-Packard; model No. 45.

TYPEWRITER Manufactured by IBM; model No. 11-¢.

X-Y PLOTTER Manufactured by Hewlett-Packard; model
No. 7890¢.

The Ge(Li) detector used in this system is of open ended coaxial pin type. The starting material for the detector is P type germanium (doped with gallium). Lithium, acting as a donor is diffused, at high temperature (400 C°) into the

cylindrical ingot creating @ thin n-type layer on the sur face. A bias voltage is used to cause the 1ithium ions to @rift through the p type material. During this process an equilibrium condition is established where lithium ions pair with atoms of the doping material (gallium) creating @ region with intrinsic properties. (See Figure §.2).

The term intrinsic implies that charge carriers will have @ very long lifetime with all recombination processes reduced to a negligible level. Under reverse bias the charge carriers can then be collected from this region re~

sulting in the production of a solid state ionization cham-

---Page Break---

fee

Lithium-Drifte

Intrinsic Region

FIGURE 5.2

(from reference 28)

---Page Break---

ber, schematically represented in Figure 5.2.

Since the mobility of lithium ions in germanium is not negligible at room temperature, such devices once fabricated, must be naintained at low temperatures to preserve the structure. A liquid nitrogen filled cryostate was used to maintain the required temperatures.

Figure 5.2 indicates the configuration of the Ge(Li) de~ tector actually used in this project.

On the average only 2.8% eV is required to create an e-

lectron-hole pair in a Go(Li) detector as compared to 30 eV in 4 gas filled ionization chamber or to 500 eV required to Produce a photoelectron at the photo cathode of a scintilla tion detector system. It is this reduced energy requirenent that improves the statistics ané thereby the resolution of

Ge(Li) detectors in comparison to gas-ionization chambers or scintillation detectors.

Th Figure §. energy vs. channel number is plotted, ine Sicating excellent 1inearity of the counting system used for Gata acquisition. Source mixtures and pertinent standares were counted within a few houre - thue reducing errors due to decay. Maximum counting registered by the inbuilt dead-time counter were below 2%. Within each counting session the gainshift remained below observable.

in order to ensure acceptable counting statistics one hour counts were taken. Countrate-outputs were obtained

both on an I8M typewriter and on an X-¥ plotter.

---Page Break---

Lithium Diffused Junction

N

4

p-Type Core

Open-ended Coaxial Ge(Li) Detector

FIGURE $.3

(from reference 28)

---Page Break---

ENERGY I ee

SYSTEM, ENERGY V5. CHANNEL WBE

308

5300 ??eoe

?OMANNEL NUMBER

FIGURE 5.4

300)

?00

---Page Break---

40

CHAPTER VI

PRESENTATION AND DISCUSSION OF RESULTS

PRCA computed results are presented in tabulated form side by side with premeasured mixing factors in order to facilitate comparison of the two. Entries in Table 6.1 re. fer to the ten-congonent simulated problem. Tables 6.2 through 6.§ contain results referring to two, three, four and five component source mixtures respectively. Discrep=

5 Of premeasured and PRCA computed mixing factors are

indicated in percents. Figures 6.1 through 6.

are samples

of pulse height distribution spectra of standard sources

and of source mixtures plotted from data obtained by the

Ge(Li) detector equipped data acquisition systen described

in Chapter ¥.

The excellent agreement between ascigned and PRGA com

Puted mixing factors in Table 6.1 indicate that the perfor-

mance of the PROA-code is essentially right. when applied

to experimentally acquired data, which by the nature of the

acquisition are affected by such factors ac gainshift, coun-

ting statistics, spectral background, etc., the discrepancy

Of premeasured and PRGA computed results - understandably

enough - increase substantially.

The PRCA computed results presented in Tables ?.2 through

6.8 are including corrections intended to compensate for er-

rors related to background, deadtime, Compton scattering and

---Page Break---

counting statistics.

Comparable published results quoted fron three referen-

ces are presented in Tables 6.6 through 6.8.

Based upon the results presented above, the following

can be concluded:

(a) The code developed can determine mixing factors of source mixtures, using gamma spectrum of the composite source as well as those of the standard sourees as input.

(b) The PRGA-code is operative on the TBM/360-40 and the DEC-10 computer both at the Computer Center of the University of Puerto Rico, Mayaguez Campus.

(©) PRGA's performance on a ten component simulated problem was found excellent.

(a) PRGA computed mixing factors have been found in satisfactory agreenent with premeasured values in @ set of measurenents performed on two, three, four and five conponent mixtures - especially prepared from reference source liquids for the purpose of this test.

(e) As indicated by entry 3 in Table 6.3,PRGA gives a near-zero mixing factor for a standard absent from the composite spectrum.

---Page Break---

COMPARISON OF ASSIGNED AND PRGA-COMPUTED MIXING FACTORS

TABLE 6.1

FOR TEN COMPONENT SIMULATED PROBLEM.

MIXING FACTORS

omponent [Assigned | PRGA Computed Discrepancy

«©

A 8.20 5.20 0.00

8 7.30 7.19 1.82

c uso 8.51 0.22

> 6.60 6.01 ous

E 20.60 10.62 e.08

F 13.80 13.82 0.07

6 1.wo awe 9.00

a 0.86 0.88 1.6

1 3.80 3.80 0.00 |

x o.us o.us 0.00

---Page Break---

TABLE 6.2

COMPARISON OF PREMEASURED AND PRGA-COMPUTED

MIXING FACTORS FOR TWO COMPONENT SOURCE MIXTURES

_MixIne_FacToRS]

SAMPLE DISCREPANCY

NUMBER | componrnr | pRca-come. | prewras. ic

aiwa?? 1.19 1.09 10-0

1

ssc5237 2.08 2.00 8.0

27087 2.35 2.5 6.0.

2

axa? 3.27 3.32 1.8

27.087 30.0 8.47 15.3

5 22

wana? 2.0 5.80 15.7

---Page Break---

TABLE 6.3

COMPARISON OF PREMEASURED AND PRGA-COMPUTED

MIXING FACTORS FOR THREE COMPONENT SOURCE MIXTURES

ee

4a

MIXING FACTORS

SAMPLE DISCREPANCY

numeer | compowryr| prempas. | proa-coup. s

aana?? 2 1.86 2.0

1 co8? 1 0.90 10.0

nS 2 2.99 a8

ana? 0.33 0.32 2.0

2 co8? 5.90 5.12 24

270° 9.38 7 23.3

aina?? 3.33 3.09 2.2

3 2700°7 2.5 2.37 5.2

270089 o 0.07 =

---Page Break---

TABLE 6.4

CORPARISON OF PRENEASURED AND PRGA-COMPUTED

MIXING FACTORS TOR FOUR COMPONENT SOURCE MIXTURES

MIXING FACTORS

SAMPLE DISCREPANCY

numpex | component __| PRENEAS[PRCA=CORE| $

aina?? 2 1.62 13.0

2stins4 1 0.38 12.0

270089 2 1.95 2.5

sscs137 2 1.60 18.0

aina?? 2 Lieu 18.0

sa 2snins* 1 0.92 8.0,

° 27¢080 2 2.35 2.5

sscgi?? 2 2.61 23.5

* Computed with w= 1/TOD

8 computed with w= 1/SQRT(TCO)

---Page Break---

TABLE 6.5

COMPARISON OF PREMEASURED AND PRGA-COMPUTED

MIXING FACTORS ToR FIVE COMPONENT SOURCE MIXTURES

>

MIXING ACTORS

SAMPLE DISCREPANCY

numpex | compouewa| prewras.| pRca-coMP. 8

ana? L 0.92 8.00

7 27C087 1 0.76 24.00

oH

25th us 9.37

27C08° 1 2.03 3.00

sscs19)| 2 der 9.50

ana? a 0.93 7.90

aa 27¢087 2 0.79 22.00

2

25rinS* sé 1.7 8.20

27¢08 a 2.03 3.00

ssost37 2 277 22.50

* Computed with w= 1/TCK)

** Computed with uj = 1/SQRTCTCK)

---Page Break---

4

TABLE 6.6

RESULTS QUOTED FROM REFERENCE

FOR TEN COMPONENT MIXTURE

~ ~ ?Quay PY

2s)

quantity

DISCREPANCY

component | premeasures | compurep $

ae? 36-8 gm 20.0 ven 3.3

ask? 0.40 mgm 0.303 mgm 25.0

25Hn56 9.202 em 0.090%yem 20.4

zise® ay.2 22.2 yen aan

aaas?® $.00 4.98 gem oe

aan

een

29cu%* 2.23 wen 211 yen 0.9

on

so

5

2ucrSt 1.82 1.86 ym =34.0

g3x128 2.49 2.68 yen 2.6

s7iat¥ 2.19 3.02 wen 37.8

uana?? | 5.00 ug 17g suo |

---Page Break---

RESULTS QUOTED FROM REFERENCE

TABLE 6.7

@

FOR THREE COMPONENT SOURCE MIXTURES

4B

MIXING FACTORS

DISCREPANCY

coMpoNEnT. easureo | compurep 8

Sacer 1 1.03 2.92

5508137 5.2 5.31 2.07

27C08 5 5.22 2s

---Page Break---

TABLE 6.8

RESULTS QUOTED FROM REFERENCE (6)

TOR FIVE COMPONENT MIXTURE

MIXING FACTORS

DISCREPANCY

component | premeasured | compurep 8

1 1 0.980 1.00

2 2 1.009 0.89

3 1 2.008 0.79

4 a 1.018 2.50

5 1 1.010 0.99

---Page Break---

COUNT RATE PER HOUR

10,000

000

100

GAMMA RAY SPECTRUM OF 37

RADIATION EMITTED BY gac

re)

CHANNEL NUMBER

FIGURE 6.2

E10 662 Mew

300 a8

---Page Break---

COUNT RATE PER HOUR

10,000

GAMMA RAY SPECTRUM OF

RADIATION EwiT TED BY C8

a a

CHANNEL NUMBER

FIGURE 6.3

720)

---Page Break---

9 3yno14

waennn TaNNEHD

sunset ed

apn" 49 o3L4ma Kouviony

40 mows 3345 A¥Y YARD

senisors

00%

?now waa aava anno

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coe ows

fom aC om caries

ono

os.

$79 3unoz4

waanw Tae

40 mnaioads Avw vaMvs

?now wad 34¥¥ LNn09

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979 gangs

w30nAN TaNNVHD

coe ozs ons,

096 090 om 0m ooo on

ETT 8

nam saziea

sanzeto-3

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?9 guns

waenAW TaNNYHD

08 008 oz ov) os om oo een

Woon 3 34¥ ANn02

a0 mnioaas Avy eMMYD

san ss90r3

ran 29003,

samo |

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9 aunord

w3ennw saNW¥HD

0% om oor cee ove om ow

gotptpa ?hase

mais ane

san 2990-3 san zziona

now waa au¥y inn0>

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Future plans include both increasing the accuracy and

extending of the scope of applicability of the PRGA-code,

The accuracy is hoped to be increased by

a) Establishing a

rary tape on which the spectra of

individual standards, obtained with very good counting

statistics, will be recorded. Whenever data on an

additional standard spectrum will become available,

1 be entered into the Library tape using an

appropriate format.

D) A baseline and gainshift routine will be added to the existing code. According to Parr and Lueas (31) even a gainshift of one channel may change results considerably.

?The scope of applicablity of PRCA is tought to be extended beyond the present one by

(2) Including a routine based on cross correlation tech~ niques for lecating peaks.

() Including an option for locating peaks enitted by the same nuclide and assigning them the came inten sity.

(e) Applying nonlinear least square fit techniques s.e. to fit experimental points to the sun of a Gaussian and a linear function.

---Page Break---

The ultimate objective in computer aided spectral decon-
Position as indicated by several authors (28, 30) is to have
@ set of activation analysis data fed to the computer and have
the computer to determine the composition of the un-irradiatea
mixture with no further man-nachine interference. Better even
have the computer continually monitor the output of the spectro
meter, computing and evaluating while the counting is in progress,
controlling the counting time, so that the sample is counted
juot long enough to get the desired statistical accuracy and
then request the system to change samples.

It is towards those very ambitious objectives that our

future research efforts will be dedicated.

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?APPENDIX,

ARRANGEMENT OF INPUT CARD DECK

FOR PRGA-CODE AND CODE LISTING

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J=

PROA-PROORAM

ARRANGEMENT OF INPUT CARD DECK FOR

PRGA - CODE.

FIGURE A.)

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PRGA-CODE LISTING

---Page Break---

zy

Fee vaeia6)

c

c

¢

7

PROGRAM... PRGA

NsKUPPUSAMY NUCLEAR ENGG, DEPT cAAM

DIMENSTON S(i@, 268)

1) +KP (268), ¥(262), +S$1G(5),D,AM(5).CC(5),Y¥ (288)

DUUBLE PRECISION? 8,1, 1rsx,ayeRSCAR~0.B AUK

THIS ?pRoGRaM ComPUTES THE? WEXING FACTORES.C(11.QY LEAST SoUARE Fl

Lf SPECTRA OF THE COMPONENTS ARE GIVEN AS INPUTS

S8(1o4) 18 THE KeTH ORDINATE OF THE T-TH SOURCE

Hie

Siw

321 FORMAT('L THE NUMBER OF COMPONENTS #tL4s/'2 THE NUMBER OF POINTS.

iy i

Ti 1S _THE NUMBER OF SPECTRA CONSIDERED ~?

ee 18 THe UNGER OF POTATS PER SBP TRON

REAQ(2 +200) (CSC 1K) e 184611) KRDO KK)

aoe PARAS SS

grecse2es ,

dee FonmAt 82 801 RY=VALUEST/79

WRITE (3+ 223) (SC 1 eK) L2de11) Keds KK)

2es Fommat(Gneyseer)

meaates sep) crea) ken

300 Fornaftare:

warte(Se883)

333 Pommard fw =vALUESI7/779

UTE ase too _

S34 FokmaT ings oree 35

EACKGROUND AND DEAQTIME CORRECTIONS OF DATA _ ao

READ(2,386)(BB(K) KEL KR)

106 FORMAT, >

READ(2. 402) TAU

402 FoRMAT(F7.2)

WaTTECS.86)

8 FORMATS VALUE OF TaUty/>

WO RRITE CS, 95) 74U, ?

95 FORMAT CAM

0-483 i=2,

00 403 Kei sKK

2.2)

SCR SSCL RCE CT RVETAUTY

SUL) 28C144) -88(K) ae

CONTINUE

00104 K=2.4

TOS ETO /L= CRYATATIY

TOR) ET CK 88K)

108 CONTINUE

COMPTON CORRECTION

HOTS waLFMroT

REAQ(2.203)HC,KKP.

203 Formati2iay

HRITEC3,89) -

9 FORMATC'a WALF WIOTH TOTAL NUMBER"OF?PEAKS1/7)

WHITECS, 90M, KP.

KREIS TOTAL NUNBER OF PEAKS =~

28) 21554805) /ACB, 5), AuxCde>, TPrve5)s RBC 288

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?S THE CHANNEL NUMBE:

READ(2, 202) (KP(K) sky

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