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NADAC AND MERGE — COMPUTER CODES FOR PROCESSING NEUTRON ACTIVATION ANALYSIS DATA

Robert E. Heft and Walter H. Martin

MASTER

May 19, 1977

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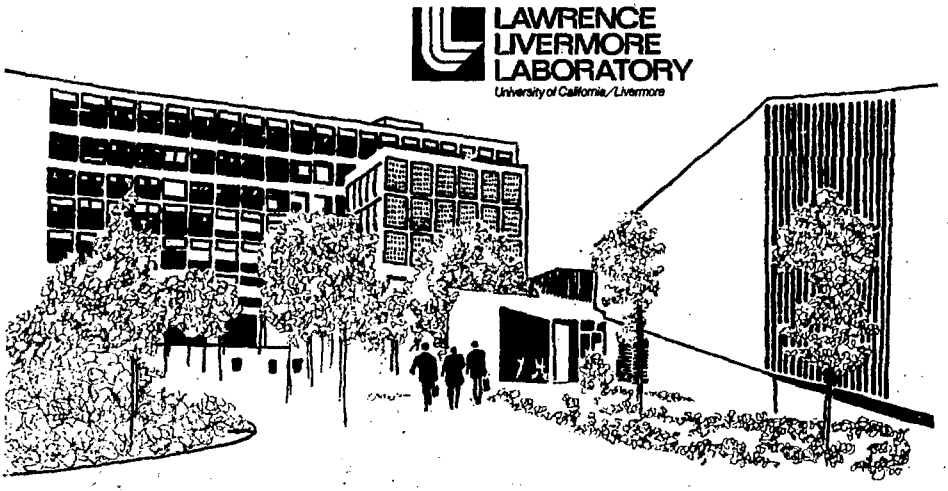

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Contents

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Abstract

Absolute disintegration rates of specific radioactive products induced by neutron irradiation of a sample are determined by spectrometric analysis of gamma-ray emissions. Nuclide identification and quantification is carried out by a complex computer code GAMANAL (described elsewhere). The output of GAMANAL is processed by NADAC, a computer code that converts the data on observed distintegration rates to data on the elemental composition of the original sample. Computations by NADAC are on an absolute basis in that stored nuclear parameters are used rather than the difference between the observed disintegration rate and the rate obtained by concurrent irradiation of elemental standards. The NADAC code provides for the computation of complex cases including those involving interrupted irradiations, parent and daughter decay situations where the daughter may also be produced independently, nuclides with very short half-lives compared to counting interval, and those involving interference by competing neutron-induced reactions. The NADAC output consists of a printed report, which summarizes analytical results, and a card-image file, which can be used as input to another computer code MERGE. The purpose of MERGE is to combine the results of multiple analyses and produce a single final answer, based on all available information, for each element found.

Introduction

The development of high-resolution systems for gamma-ray spectrometry and of computer codes for quantitative analysis of the radionuclides in spectral constituents has made feasible the routine use of "instrumental neutron activation analysis" (INAA) for determining the elemental composition of complex samples. The Environmental Research Division of Lawrence Livermore Laboratory has used INAA for the analysis of samples from a variety of environmental programs. Two computer codes, NADAC and MERGE, were developed for processing INAA data. The gamma-ray spectral data on the activated samples are processed by GAMANAL, a spectral resolution code developed by R. Gunnink and J. Niday.[1]

NADAC, the "neutron activation data analysis code" described in this report, converts the disintegration-rate data provided by GAMANAL to elemental

abundance values. NADAC uses an absolute computational method based on neutron cross sections and radioactive-decay rates. The code provides the correct calculation of elemental abundance (total micrograms) even when:

- Counting time is long compared to half-life of radionuclide being counted.
- Sample is subjected to multiple or interrupted irradiations.
- Nuclide counted is daugher of nuclide produced, including the case where daughter is also produced independently.
- Radionuclide produced by (n, γ) reaction on element of interest is also produced by (n, f) or (n, p) reaction on a different element.

For computing net concentrations of the elements, the input to NADAC consists of the resolved spectral data obtained from all sample counts from a given irradiation, the necessary information on the sample itself, and data on the concentrations of the elements in the materials used for collection of samples (materials blanks). The NADAC output is in the form of printed tables for each sample which list the total micrograms for each element present, for the materials blanks, and for the micrograms resulting from (n, p) or (n, f) interference. Finally, the net micrograms of each element per unit amount of sample is listed. The net is obtained after materials-blank and interference-blank corrections. In addition, a second output file is generated, in a card format, which simply lists for each sample the net micrograms of each element per unit amount of sample.

For replicate samples or samples subjected to more than one irradiation (e.g., a short and a long irradiation), the results are combined by means of a companion code MERGE, and a weighted mean is obtained from the inverse square of the standard deviation. The MERGE input consists of the card-format output files of NADAC for the sample set. MERGE can also be used to combine results from analyses by other methods (e.g., x-ray fluorescence or atomic absorption), providing the data are in the NADAC card format. The output of MERGE also consists of two files: a printed output with titles, which lists the elemental concentrations found for each sample and their weighted mean values; and a card-format output, which gives for each sample the weighted mean value of the concentration of each element as well as a sample description, the latter being provided by the individual requesting the analyses.

In the following, we describe the operation of NADAC and MERGE in sufficient detail so a reader starting from bare files can independently operate the codes. To make our description specific, we have included, as examples, the input and output files for a particular group of samples that were subjected to both short and long irradiations and were subsequently counted at various times.

Description of the Analytical Procedure

Particulate matter from a known volume of air was collected on filters and on impactor stages. The object was to determine the concentrations of the elements in the air (micrograms/standard cubic foot). For long irradiations, a sample set for collection and analysis consisted of eight filter units, four impactor stages, and two small pieces of aluminum for collecting cesium deposits and determining micrograms of cesium per sample. Based on previous irradiations of filter and impactor materials alone, data on the concentrations of elements in these blanks were available. The filter samples were divided into two groups; one set of four samples was counted in the polyethylene bags in which they were irradiated. Blank data for the polyethylene were also available.

For short irradiations, a sample set consisted of the eight filter units and four impactor stages described above and also two small filters. On each of the latter, 60.0 μg of Mn was deposited. The Mn standards were subjected to a single count of 40-min duration. The two cesium samples were not used in short irradiations. The eight filter samples were divided into two groups of four as above and were irradiated for 1 min and counted after approximately 10 min of cooling. The four impactors were irradiated for 5 min and counted after a 10-min cooling period. All of these filter and impactor samples were given 3 consecutive counts of 10, 20, and 40 min.

Nineteen days after short-irradiation runs, the 14 samples as well as 2 multi-element standards were irradiated for 72 min and counted twice: an 8,000-sec count after cooling for 3 days and a 20,000-sec count after cooling for 15 days.

All spectra from the long and short irradiations were analyzed by GAMANAL. The output consisted of one set of GAMANAL cards for the short and one set for the long irradiations. Each card gave the absolute disintegration rate for a single radionuclide from a given count of a given sample. NADAC combined

disintegration rate data with other experimental and descriptive parameters in order to compute and report the net micrograms of an element in a given amount of sample. The NADAC results for the two irradiations were combined by MERGE.

Figure 1 shows an overview flow chart of the NADAC program. The six input files presented to NADAC are shown in the order they appear in the Execute Command. The three files that carry the suffix "LIB" are semipermanent files and carry over from irradiation to irradiation. In a single NADAC run, data is processed from one or more irradiations (files that apply only to the irradiations carry the suffix "FILE" in Fig. 1). In actual operation of the code, the order of listing of the files is important; however, file names can be arbitrarily assigned. In the following, we describe the format and content of the input files in order of their presentation to NADAC. For NADAC to run, all files except the flux monitor file (FM FILE) must be present. The FM FILE is optional.

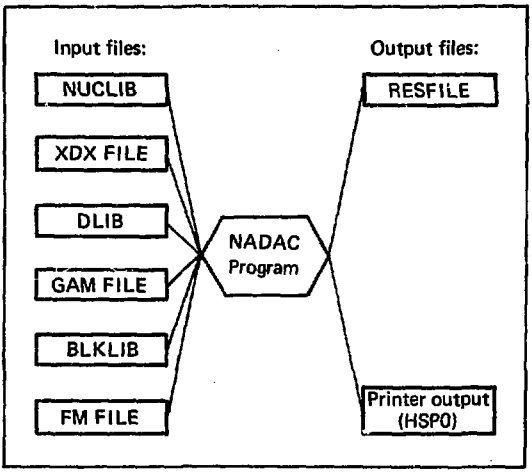

Fig. 1. Overview flow chart for NADAC.

NADAC Input Files

NUCLIB FILE

The NUCLIB file contains all the nuclear parameters required for the calculations. The file consists of one card for each nuclide and is ordered by their atomic number and atomic mass. Nuclides found by GAMANAL but not included in the NUCLIB file will be ignored by NADAC. Maximum file length is 200 cards. An abridged example of a NUCLIB file is shown in Fig. 2.

```
11024  NA 1.000E+00 6.250E-01 8.604E+06 0.          0.          1.000E+00
12027  MG 1.000E+00 6.597E-03 6.533E+04 1.700E-01  0.          1.000E+00 13028
13026  AL 1.000E+00 1.597E-03 3.211E+05 0.         0.          1.000E+00
17038  CL 1.000E+00 2.690E-02 1.110E+06 0.         0.          1.000E+00
19042   K 1.000E+00 5.150E-01 1.005E+06 0.         0.          1.000E+00
20047  CA 1.000E+00 4.540E+00 2.204E+02 0.        -0.          1.000E+00
20049  CA 1.000E+00 6.042E-03 1.651E+04 0.         0.          1.000E+00
21045  SC 1.000E+00 8.390E+01 2.182E+06 0.        -0.          1.000E+00
22051  TI 1.000E+00 4.028E-03 7.429E+04 0.         0.          1.000E+00
23052   V 1.000E+00 2.604E-03 3.548E+07 0.         0.          1.000E+00
24051  CR 1.000E+00 2.772E+01 5.159E+06 0.        -0.          1.000E+00
25056  MN 1.000E+00 1.074E-01 9.559E+07 0.         0.          1.000E+00
26059  FE 1.000E+00 4.460E+01 2.546E+04 0.        -0.          1.000E+00
27058  NI 1.000E+00 7.190E+01 8.019E+04 0.        -0.          1.000E+00
27060  CO 1.000E+00 1.922E+03 2.426E+08 0.        -0.          1.000E+00
28065  NI 1.000E+00 1.060E-01 1.089E+05 0.         0.          1.000E+00 29066
29064  CU 1.000E+00 5.330E-01 1.830E+07 0.         0.          1.000E+00 30369
29066  CU 1.000E+00 3.842E-03 4.076E+06 0.         0.          1.000E+00 30369
30065  ZN 1.000E+00 2.486E+02 2.246E+08 0.        -0.          1.000E+00
30369  ZN 1.000E+00 5.933E-01 8.246E+04 0.         0.          1.000E+00
31072  GA 1.000E+00 5.083E-01 1.194E+07 0.         0.          1.000E+00
33075  AS 1.000E+00 1.096E+00 2.865E+07 0.        -0.          1.000E+00
34075  SE 1.000E+00 1.200E+02 2.714E+06 0.        -0.          1.000E+00
35080  BR 1.840E-01 1.222E-02 9.087E+06 0.         1.613E+01 3.160E+00
35082  BR 4.236E-03 1.473E+00 8.750E+06 0.        -8.294E-06 1.114E+00
35380  BR 1.000E+00 1.840E-01 9.087E+06 0.         0.          1.000E+00
37086  RB 1.000E+00 1.866E+01 2.027E+06 0.        -0.          1.000E+00
38085  SR 1.000E+00 6.519E+01 2.877E+04 0.        -0.          1.000E+00
38385  SR 1.000E+00 4.823E-02 2.132E+04 0.         0.          1.000E+00
38387  SR 1.000E+00 1.171E-01 3.965E+05 0.         0.          1.000E+00
40095  ZR 1.000E+00 6.500E+01 6.721E+04 6.262E+00-0.          1.000E+00 93239
40097  ZR 1.000E+00 7.000E-01 6.794E+03 5.585E+01  0.          1.000E+00 93239
42099  MO 1.000E+00 2.752E+00 4.195E+05 9.493E-01-0.          1.000E+00 93239
47410  AG 1.000E+00 2.530E+02 1.016E+07 0.        -0.          1.000E+00
48115  CD 1.000E+00 2.208E+00 6.672E+05 1.689E-03-0.          1.000E+00 93239
49416  IN 1.000E+00 3.774E-02 8.036E+08 0.         0.          1.000E+00
51122  SB 1.000E+00 2.760E+00 2.245E+07 0.        -0.          1.000E+00
51124  SB 1.000E+00 6.030E+01 1.004E+07 0.        -0.          1.000E+00
```

Fig. 2. Abridged NUCLIB file.

NUCLIB Card Description

The description (see listing below) includes the card fields (specified by column numbers), the mnemonic name (in capital letters) used in NADAC, the format specification for the field (in parentheses), and a definition of the parameter.

Column No.	Mnemonic (Format)	Description
2-6	NUC (R5)	Nuclide code ZZAAA (e.g., 11024 = ^{24}Na). The GAMANAL convention of indicating metastable states by adding 300 to mass (e.g., 63452 = ^{152}Eu) is followed.
9-10	SS (R2)	Chemical symbol of target element (right-adjusted for those elements having single-letter symbols).
11-20	TPAR (E10.0)	Parent half-life in days. If radioactive product has no parent, a value of 1.000 E + 00 is entered.
21-30	TDAU (E10.0)	Half-life in days of daugher or, if radioactive product is directly produced, of product nuclide.
31-40	RATE (E10.0)	The rate of production of parent or of directly produced product nucleus, expressed as atoms/min/μg at a flux of 1×10^{13} neutrons/cm^2/sec. The determination of rate constant from nuclear data is described in section on NADAC computations.*
41-50	FTR (E10.0)	The numerical value of the interference-blank correction. This value multiplies the total micrograms of element, indicated by nuclide code listed in Cols. 72-76, to arrive at (n, p) or (n, f) contribution to total micrograms found.*
51-60	KPAR (E10.0)	A constant used in calculating total micrograms. If there is a parent-daughter pair, KPAR = $\frac{TPAR}{TPAR - TDAU} + \frac{TPAR}{TDAU}$. Otherwise, KPAR = 0.
61-70	KDAU (E10.0)	A constant used in calculating total micrograms. If there is a parent-daughter pair, KDAU = $1 - \frac{TPAR}{TPAR - TDAU} + \frac{\sigma_D}{f\sigma_p}$. Otherwise, KDAU = 1.000E + 00. Here, σ_D and σ_p are thermal neutron activation cross sections of daughter and parent, respectively, and f is fraction of parent decays leading to daughter.
71-60	NUX (R6)	Nuclide code (ZZAAA) of element which produces interfering (n, p) or (n, f) reaction.

*Both RATE and FTR values for the individual nuclides are dependent on their irradiation location within the reactor. NADAC has a built-in capability for modifying these factors during the course of the computation (discussed below under NUCGEN auxiliary program).

XDX FILE (CROSS-INDEX)

The XDX file consists of one card for each irradiated sample. Each card relates an irradiation descriptor code with a sample descriptor code and provides for the entry into NADAC of sample size and information from the control blanks and flux monitor. The maximum file length is 200 lines.

The XDX file for the samples described previously is shown in Fig. 3. The irradiation descriptor code for the long irradiation is 22[illegible], while the codes for the three companion short irradiations are B87, B88 and B89. Within an irradiation group, the XDX cards must be arranged in the same order as that of the samples and standards during irradiation.

```
[illegible]  14 1.000E+00  08 4.5                    2.679  0.75
[illegible]  13 1.000E+00  0217.35 0495.0
[illegible]  13 1.000E+00  0217.35 0495.0
[illegible]  13 1.000E+00  0217.35 0495.0
[illegible]  13 1.000E+00  0217.35 0495.0
[illegible]  13 1.000E+00  0217.35
[illegible]  13 1.000E+00  0217.35
[illegible]  13 1.000E+00  0217.35
[illegible]  13 1.000E+00  0217.35
[illegible]  13 1.000E+00  0517.35
[illegible]  13 1.000E+00  0521.61
[illegible]  13 1.000E+00  0521.61
[illegible]  13 1.000E+00  0521.61
[illegible]  14 1.000E+00
[illegible]  14 1.000E+00
[illegible]  14 1.000E+00  08 4.5                    2.664  0.94
[illegible]  14 1.000E+00  08 2.3                    2.287  0.65
[illegible]  13 1.000E+00  0217.35 0495.0           2.287  0.65
[illegible]  13 1.000E+00  0217.35 0495.0           2.287  0.65
[illegible]  13 1.000E+00  0217.35 0495.0           2.287  0.65
[illegible]  13 1.000E+00  0217.35 0495.0           2.287  0.65
[illegible]  14 1.000E+00  08 2.3                    2.287  0.90
[illegible]  14 1.000E+00  08 2.3                    2.259  0.90
[illegible]  13 1.000E+00  0217.35                   2.259  0.90
[illegible]  13 1.000E+00  0217.35                   2.259  0.90
[illegible]  13 1.000E+00  0217.35                   2.259  0.90
[illegible]  13 1.000E+00  0217.35                   2.259  0.90
[illegible]  14 1.000E+00  08 2.3                    2.259  0.90
[illegible]  14 1.000E+00  08 2.3                    2.251  1.05
[illegible]  13 1.000E+00  0517.35                   2.251  1.05
[illegible]  13 1.000E+00  0521.61                   2.251  1.05
[illegible]  13 1.000E+00  0521.61                   2.251  1.05
[illegible]  13 1.000E+00  0521.61                   2.251  1.05
[illegible]  14 1.000E+00  08 2.3                    2.251  1.05
```

Fig. 3. XDX file.

XDX Card Description

Column No.	Mnemonic (Format)	Description
1	X	Card-type indicator not read by NADAC.
2-7	IRX (R6)	Irradiation descriptor code. Three-digit irradiation number followed by three-digit sample number. Alphabetic symbols may be used.
8-10	XTYP (R3)	Sample-type descriptor code. Usually a three-letter combination.

Column No.	Mnemonic (Format)	Description
11-16	SPL (R6)	Sample number. Three-digit sample number followed by three digits that are optional and can be used to number replicates.
18-19	MUF (I2)	Mass units code. Final answers are reported as micrograms per "mass unit". This code, which is permanently stored in NADAC, controls title selection and inserts for "mass unit", the quantity indicated in Table 1. Columns 51-70 of the DLIB card provide information for converting to units selected by experimenter.
21-29	MASS (E10.0)	Sample amount, defined by mass units code of Cols. 18-19 (see Table 1).

The following entries are optional:

31-34	FSD (F5.0)	Fractional standard deviation of sample amount.
36-37	BL1 (I2)	Materials-blank code for first blank material. Selects appropriate column of blank library for calculating corrections for blank. Also, controls title selection in accordance with library list of blank materials. Blank code for particular material is specified in BLKLIB as described below.
38-42	MLT1 (F5.0)	Multiplier for first blank. MLT1 is simply the amount of blank material used in the sample being analyzed. Blank library data are entered as nanograms per unit of material. The unit can be mg, gm, cm^2, or whatever units are appropriate.
44-45	BL2 (I2)	Materials-blank code for second blank material. Thus, in line 2 of Fig. 3, a 17.35 cm^2-impactor stage was contained in a 95.0 mg polyethylene bag. The blank data for the impactor stage was contained in Col. 02 of the blank library, and that for the polyethylene bag in Col. 04.
46-50	MLT2 (F5.0)	Multiplier for second blank.
52-60	FMMS (E10.0)	Mass of flux monitor in micrograms. As indicated earlier, the use of a flux monitor file (FMFILE) is optional in NADAC, but if used, the mass of the flux monitor is entered in the XDX file at this point.

Column No.	Mnemonic (Format)	Description
62-67	PHIFM (F6.0)	Flux factor. Thermal neutron flux expressed as 10^{13} neutrons/cm^2/sec. An externally determined flux factor can be used in lieu of the internal flux monitor file. NADAC will use the PHIFM values given for each sample and will do a linear interpolation for missing values. See treatment of flux factor under NADAC computations.
69-72	PSXFM (F4.0)	Percent standard deviation of PHIFM.

Table 1. Mass units code used in NADAC and MERGE.

Mass Code	Abbreviation	Remarks
01	GM	Gram.
02	GM ASH	Gram of ash.
03	GM DRY	Gram of dry weight (usually used for freeze-dried material).
04	GM WET	Gram of wet weight.
05	KG	Kilogram.
06	KG DRY	Kilogram of dry weight.
07	KG WET	Kilogram of wet weight.
08	MG	Milligram.
09	LITER	Liter.
10	ML	Milliliter.
11	SQ CM	Square centimeter.
12	SCF	Standard cubic foot, a cubic foot of air at standard temperature and pressure (STP).
13	STAGE	One stage of an impactor, for example.
14	SAMPLE	---
15	CU METER	Cubic meter.
16	VVVV	16 through 20 provide for future additions to table.
17	WWWW	
18	XXXX	
19	YYYY	
20	ZZZZ	

DLIB FILE (SAMPLE DESCRIPTION FILE)

The DLIB file consists of one card for each sample. Each card associates the six-symbol, sample descriptor code with a more extensive sample description and, as an option, provides the information necessary for converting the units used in the analytical results. Thus, if the analysis ordinarily produces answers in micrograms of element per gram of ash, these can be converted to the corresponding per gram wet weight if the appropriate ratio of wet weight to ash weight is entered on the DLIB card. The extended descriptive portion of the DLIB card is used in the NADAC code for title selection. DLIB is also used in the MERGE code, and the extended description appears in the final output file of MERGE as a label assigned to each elemental, analytical result.

Although, a DLIB file must be included for NADAC (and MERGE) to run, the card describing a particular sample can be missing. In this case, the codes use a "No Descriptive Data" message in the output files. The samples listed in the DLIB may be for more than one irradiation. The maximum number of lines in DLIB is 1,000. A partial listing of a DLIB file is shown in Fig. 4.

```
DRCD100 FC03IMPC  MK3037 01C 01A 08:45 760223     13 12 0.371E+00
DRCD101 FC03IMPC  MK3037 02C 01A 08:45 760223     13 12 0.371E+00
DRCD102 FC03IMPC  MK3037 03C 01A 08:45 760223     13 12 0.371E+00
DRCD103 FC03IMPC  MK3037 04C 01A 08:45 760223     13 12 0.371E+00
DRCD104 FC03IMPC  MK3037 05C 01A 08:45 760223     13 12 0.371E+00
DRCD105 FC03IMPC  MK3037 06C 01A 08:45 760223     13 12 0.371E+00
DRCD106 FC03IMPC  MK3037 07C 01A 08:45 760223     13 12 0.371E+00
DRCD107 FC03IMPC  MK3037 08C 01A 08:45 760223     13 12 0.371E+00
DRCD108 FC03IMPC  MK3031 01C 04  08:40 760219     13 12 1.56 E+00
DRCD109 FC03IMPC  MK3031 02C 04  08:40 760219     13 12 1.56 E+00
DRCD110 FC03IMPC  MK3031 03C 04  08:40 760219     13 12 1.56 E+00
DRCD111 FC03IMPC  MK3031 04C 04  08:40 760219     13 12 1.56 E+00
DRCD112 FC03IMPC  MK3031 05C 04  08:40 760219     13 12 1.56 E+00
DRCD113 FC03IMPC  MK3031 06C 04  08:40 760219     13 12 1.56 E+00
DRCD114 FC03IMPC  MK3031 07C 04  08:40 760219     13 12 1.56 E+00
DRCD115 FC03IMPC  MK3031 08C 04  08:40 760219     13 12 1.56 E+00
DRCD116 FC03IMPC  MK3033 01C 04  11:30 760219     13 12 1.27 E+00
DRCD117 FC03IMPC  MK3033 02C 04  11:30 760219     13 12 1.27 E+00
DRCD118 FC03IMPC  MK3033 03C 04  11:30 760219     13 12 1.27 E+00
DRCD119 FC03IMPC  MK3033 04C 04  11:30 760219     13 12 1.27 E+00
DRCD120 FC03IMPC  MK3033 05C 04  11:30 760219     13 12 1.27 E+00
DRCH020 FC03FILTERN  020      14  14:35 760210     13 12 0.595E+00
DRCH025 FC03FILTERN  025      04  14:45 760209     13 12 1.06 E+00
DRCH026 FC03FILTERN  026      04  15:30 760209     13 12 0.80 E+00
DRCH028 FC03FILTER   028      04  09:40 760213     13 12 2.56 E+00
DRCH030 FC03FILTER   030      04  10:30 760213     13 12 0.07 E+00
DRCH045 FC03FILTERN  045      04  08:45 760218     13 12 5.910E+00
DRCH046 FC03FILTERN  046      04  10:15 760218     13 12 2.610E+00
DRCH047 FC03FILTERN  047      01A 08:15 760218     13 12 5.100E+00
DRCH048 FC03FILTERN  048      01A 09:30 760218     13 12 4.990E+00
DRCH049 FC03FILTERN  049      04  11:00 760218     13 12 2.830E+00
DRCH050 FC03FILTERN  050      01A 10:30 760218     13 12 6.310E+00
DRCH051 FC03FILTERN  051      04  11:30 760218     13 12 2.860E+00
DRCH052 FC03FILTER   052      01A 08:54 760219     13 12 2.02 E+00
DRCH053 FC03FILTER   053      04  08:20 760219     13 12 2.49 E+00
DRCH054 FC03FILTER   054      04  09:20 760219     13 12 0.44 E+00
DRCH055 FC03FILTERN  055      04  09:35 760219     13 12 4.000E-01
DRCH056 FC03FILTERN  056      01A 10:10 760219     13 12 5.010E+00
```

Fig. 4. Abridged DLIB file.

DLIB Card Description

Column No.	Mnemonic (Format)	Description
1	D	Card-type indicator not read by NADAC.
2-7	NCOD (R6)	Sample descriptor code. Usually a combination of three-letters and three-numbers. To identify the sample, NADAC looks for a match between NCOD and Cols. 8-13 of the X card.
9-45	Free field (3R10 +A7) ND1, ND2, ND3, ND4	Descriptive data furnished by experimenter who requests analyses.
51-52	MCU (I2)	Mass code used. If this matches MUF entry on X card, a switch will be made in the units in which results are reported.
54-55	MCW (I2)	Mass code wanted. Mass code for units in which results will be reported.
57-65	FMASS (E9.0)	Ratio of units wanted to units used.
67-70	FSDM (F4.0)	Fractional standard deviation of FMASS.

GAMFILE

GAMFILE is made up of Z-cards, which give irradiation time data for a particular set of samples having a common irradiation history, and GAMANAL cards for this set. The GAMANAL cards include all the counts made on these samples and are in a GAMANAL-controlled format that is specified for activation analysis [Entry of "5" in Col. 71 of GAMANAL-2-card]. If desired, a complete GAMFILE can hold several Z-card/GAMANAL-card data sets covering more than one irradiation. Within such a group, the GAMANAL cards from a single count must be kept together; however, NADAC sorts the separate counts so the order of their presentation is not critical. The maximum file length of a GAMFILE is 1,000 lines plus the number of Z-cards used. A partial GAMFILE listing is shown in Fig. 5.

GAMFILE Z-Card Description (See Fig. 6 for irradiation- and counting-time periods).

Column No.	Mnemonic (Format)	Description
1	Z (R1)	NADAC reads the GAMFILE one card at a time. When a Z-card is encountered, zero time is reset, and certain parameters that depend on irradiation history are recomputed.

2-4	Not used (I3)	Irradiation code.
6-8	DAY (I3)	Day of year (001-365) when final irradiation was completed.
10-15	TZERO (R6)	Time of completion of final irradiation, expressed as HHMMSS, where HH = hours, MM = minutes, SS = seconds. Based on a 24-hour clock (e.g., 131000 = 1:10 p.m.).
16-23		Not used here; however, see NUCGEN.
24-29	TAU1 (R6)	Time in reactor for final irradiation, expressed as HHMMSS (e.g., for an irradiation of 4 h, 10 min, 30 sec, TAU1 = 041030).
30-36	DEL2 (R7)	Interval between completion times of final irradiation and previous one, expressed as DDDHHMM (see Fig. 6).
38-43	TAU2 (R6)	Time in reactor for the next to the last irradiation, expressed as HHMMSS and adjusted for relative flux of the next to the last and the final irradiations. Where the next to the last irradiation was for 60 sec but flux was only 80% of that in final irradiation, the time in reactor is taken as 80% of 60 sec or 48 sec.
44-50	DEL3 (R7)	Interval between completion times of final irradiation and τ_3 irradiation (see Fig. 6), expressed as DDDHHMMM.
52-57	TAU3 (R6)	Time in reactor for τ_3 irradiation, expressed as HHMMSS and adjusted for relative flux.

GAMFILE GAMANAL Card Description

The card put out by GAMANAL for neutron activation is a general purpose card and contains some information not used by NADAC.

Column No.	Mnemonic (Format)	Description
1-5	IRG (R5)	Nuclide code ZZAAA (11024 = ^{24}Na).
6-15	Not used (E10.3)	Disintegration rate (DPM) of IRG at zero time. Not used because GAMANAL algorithm for parent-daughter pairs assumes zero daughter at zero time. Does not allow for daughter growth during irradiation.

```
2221 219 162537          00720039041370 00004B
11024 1.664E+09   2.5 RCH2210011     8000 222.6778   3  5.[illegible]  733
19042 1.398E+08  31.7 RCH2210011     8000 222.6778   3  2.[illegible]  734
21046 4.691E+05   6.8 RCH2210011     8000 222.6778   3  4.[illegible]  735
26059 2.184E+05  27.1 RCH2210011     8000 222.6778   3  2.[illegible]  736
31072 1.755E+07   7.2 RCH2210011     8000 222.6778   3  4.[illegible]  737
20047 1.501E+04  20.9 RCH2210012    20000 233.6126  14  1.[illegible]   29
21046 4.217E+05   1.0 RCH2210012    20000 233.6126  14  3.[illegible]   30
24051 9.464E+04   2.4 RCH2210012    20000 233.6126  14  6.[illegible]   31
25054 5.928E+03   4.0 RCH2210012    20000 233.6126  14  5.[illegible]   32
26059 1.892E+05   1.1 RCH2210012    20000 233.6126  14  1.[illegible]   33
11024 2.346E+09   5.1 RCH2210021     8000 222.7754   3  7.[illegible]  750
19042 1.925E+08  13.4 RCH2210021     8000 222.7754   3  2.[illegible]  751
21046 4.822E+05   7.5 RCH2210021     8000 222.7754   3  4.[illegible]  752
31072 1.908E+07   7.5 RCH2210021     8000 222.7754   3  4.[illegible]  753
33076 1.041E+07   5.7 RCH2210021     8000 222.7754   3  1.[illegible]  754
21046 4.951E+05   1.2 RCH2210022    20000 233.8550  14  4.[illegible]   69
24051 1.746E+05   2.3 RCH2210022    20000 233.8550  14  1.[illegible]   70
25054 6.603E+03   3.4 RCH2210022    20000 233.8550  14  6.[illegible]   71
26059 2.084E+05   1.9 RCH2210022    20000 233.8550  14  1.[illegible]   72
27058 6.812E+02  33.7 RCH2210022    20000 233.8550  14  5.[illegible]   73
2221 219 162537          00720038857370 00004B
11024 1.515E+07   5.3 RCH2210051     8000 223.0662   3  3.[illegible]  163
19042 3.981E+05  37.1 RCH2210051     8000 223.0662   3  3.[illegible]  164
20047 6.449E+02  22.7 RCH2210051     8000 223.0662   3  3.[illegible]  165
21046 1.160E+03  15.1 RCH2210051     8000 223.0662   3  1.[illegible]  166
24051 2.381E+04   4.7 RCH2210051     8000 223.0662   3  2.[illegible]  167
24051 2.483E+04   1.3 RCH2210052    20000 234.5676  14  1.[illegible]  182
25054 3.867E+01  31.6 RCH2210052    20000 234.5676  14  3.[illegible]  183
26059 1.173E+03   3.9 RCH2210052    20000 234.5676  14  9.[illegible]  184
27060 1.698E+02   7.4 RCH2210052    20000 234.5676  14  1.[illegible]  185
30065 5.780E+02   8.2 RCH2210052    20000 234.5676  14  5.[illegible]  186
11024 7.776E+07   5.8 RCH2210061     8000 223.1631   3  1.[illegible]  188
19042 1.567E+06  32.6 RCH2210061     8000 223.1631   3  1.[illegible]  189
21046 3.635E+03  19.1 RCH2210061     8000 223.1631   3  3.[illegible]  190
24051 7.022E+04   6.3 RCH2210061     8000 223.1631   3  6.[illegible]  191
31072 9.682E+05   5.2 RCH2210061     8000 223.1631   3  1.[illegible]  192
20047 1.181E+03  10.0 RCH2210062    20000 234.8003  15  1.[illegible]    2
21046 3.604E+03   2.1 RCH2210062    20000 234.8003  15  3.[illegible]    3
24051 7.262E+04   0.9 RCH2210062    20000 234.8003  15  4.[illegible]    4
25054 1.022E+02  25.1 RCH2210062    20000 234.8003  15  9.[illegible]    5
26059 3.652E+03   2.8 RCH2210062    20000 234.8003  15  3.[illegible]    6
```

Fig. 5. Abridged GAMANAL file.

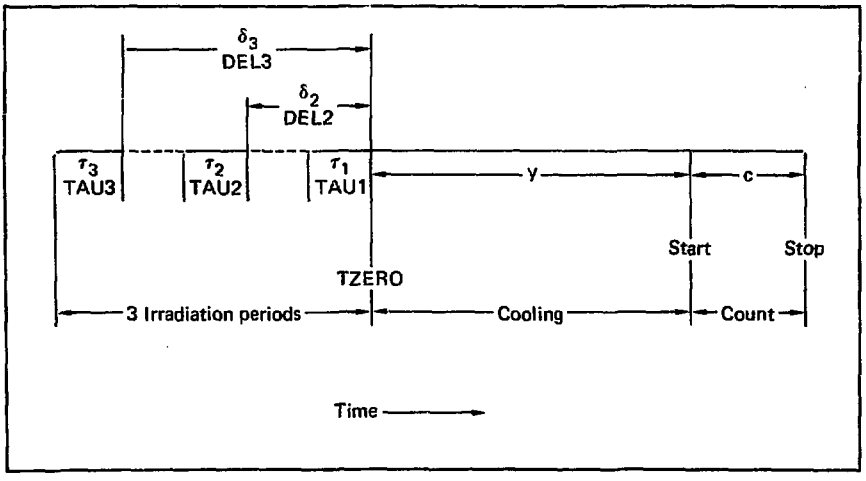

Fig. 6. Irradiation, cooling, and counting times.

Column No.	Mnemonic (Format)	Description
17-20	PSD (F5.0)	Percent standard deviation of DPM of IRG at zero time and at count time.
22-39	See following listing	Information in Cols. 22-39 of GAMANAL output card is entered into GAMANAL as Cols. 2-19 of the GAMANAL Type 2 input card.
22-24	TYP (R3)	Sample type descriptor code. NADAC looks for match with XTYP, Cols. 8-10 of XDX file, for the irradiation code given below. Failure to match causes NADAC to skip sample.
25-30	IRRC (R6)	Irradiation descriptor code. Seeks match with IRX, Cols. 2-7 in XDX card file, to obtain related data for sample.
31	LNUM (R1)	Sequence number of counts following last irradiation. For first count LNUM = 1, for second count LNUM = 2, etc. Used in sorting and tabulation and must be included.
32-34	T1 (I3)	Last three decimal places of time of day at start of count, expressed as a decimal fraction to six places. See TST below.
35-39	T2 (I5)	Real-time duration of count, expressed in seconds.
40-47	TST (F8.0)	Time the count was started, expressed as day of year plus decimal fraction of day, and entered on GAMANAL-2 card to nearest one-thousandth of a calendar day. However, 0.001 day is 1.44 minutes, which is not sufficiently accurate for half-lives that range in minutes. For spectra of short irradiations, three additional decimal places are carried by listing them as T1 in Cols. 32-34, as noted above.
54-64	DPMCT (E11.0)	Disintegration rate, expressed as DPM at count time. This is number of disintegrations divided by live-time of analyzer.
65-70	SPEC (R6)	Spectrum identification number.
71-72	CTR (R2)	Identification number for spectrometer system used for gamma-ray analysis.

BLKLIB FILE

The BLKLIB File carries information on the materials blanks for up to ten materials and consists of a pair of cards for each nuclide for which a blank correction is required. On the first card, the nuclide number is followed by 10 columns of data (one for each material), which give the quantity

for a blank, expressed as nanograms per unit amount of each material. On the second card the nuclide number is followed by the fractional standard deviation of the amount for each blank. At the end of the set of card pairs, a single unpunched card is inserted. This is followed by a series of ten cards (corresponding to the ten columns) each of which describes one of the blank materials and states the units used in expressing the amount of the blank. An abridged listing of a BLKLIB File is shown in Fig. 7.

```
11024    5.46    263.3    14.7    15.0    10.8    0.    132.    211.    1500.    0.
11024     .02     .10      .91     .07     .20    0.     .21     .22      .25     0.
12027    92.0     0.       0.      0.      0.     0.     0.      0.       0.      0.
12027     .24     0.       0.      0.      0.     0.     0.      0.       0.      0.
13028    41.0     0.       0.     15.0    7.6     0.     0.     62.4    13765.    0.
13028     .45     0.       0.      .02     .20    0.     0.      .21      .54     0.
17038    158.     370.0    0.     3.05    176.    0.     0.     407.     2113.    0.
17038     .21     .14      0.      .06     .06    0.     0.      .20      .23     0.
19042     .194    0.       6.1    4.4     20.     0.     31.     0.      2100.    0.
19042     .26     0.       .27    .26     .14    0.     .40     0.       .22     0.
20047    176.     0.       0.     0.      0.     0.     0.     70.       0.      0.
20047     .41     0.       0.     0.      0.     0.     0.      .20      0.      0.
20049    176.     0.       0.     0.      0.     0.     0.     70.       0.      0.
20049     .41     0.       0.     0.      0.     0.     0.      .20      0.      0.
21046     .0005   .0021    .0021  .0033   .0066  0.     0.      .01      .97     0.
21046     .11     .34      .34    .10     .10    0.     0.      .12      .12     0.
22051     .36     0.       .36   1.00     0.     0.     0.     0.0       0.      0.
22051     .04     0.       .34    .05     0.     0.     0.     0.0       0.      0.
23052             0.              .132    0.
23052             0.              .08     0.
24051     .99     6.46     0.     .174    1.24   0.     .73    1.46     89.     0.
24051     .11     .30      0.     .12     .07    0.     .10     .10      .10     0.
25056     .82     .171     .36    .051    .34    0.     0.     1.60     43.9     0.
25056     .74     .30      .50    .05     .27    0.     0.      .56      .21     0.

 1 AVICEL                MG
 2 NUCLEOPORE            SQ CM
 3 KEMFOL                SQ CM
 4 POLY BAG              MG
 5 COATED KEMFOL         SQ CM
 6 EMPTY
 7 FORMADEHYDE           GM MILK
 8 WHATMAN-41            SQ CM
 9 POLYETHYLENE            GM
10 NONE                    NONE
```

Fig. 7. Abridged BLKLIB file.

BLKLIB Data Cards

Column No.	Mnemonic (Format)	Description
Odd-numbered cards:		
1-5	BLKZA (R5)	Nuclide Code ZZAAA (line 1-11024).
6-76	BLK_I (I=1,10) (10F7.0)	Nanograms per unit amount of blank for each of 10 materials (e.g., Fig. 6, line 1: 5.46, 263.3, etc.).

Column No.	Mnemonic (Format)	Description
Even-numbered cards:		
1-5	FSDZA (R5)	Nuclide code ZZAAA (line 2-11024).
6-76	BLR_I (I=1,10) (10F7.0)	Fractional standard deviation of nanograms per unit amount of blank for each of 10 materials (e.g., Fig. 6, line 2: 0.02, 0.01, etc.).

BLKLIB Descriptor Cards

Column No.	Mnemonic (Format)	Description
3-4	Blank number (R2)	Blank number (1-10) is not read by NADAC.
5-24	ID1, ID2 (2R10)	Blank material description used in titles.
25-34	IU (R10)	Blank-amount units used in titles and as reminder to user of BLKLIB.

FMFILE (FLUX MONITOR FILE)

All the previously described files, whether or not they contain information relative to the particular sample set, must be available to NADAC in order for it to run. Whether or not blank corrections are needed or descriptive data is desired, BLKLIB and DLIB files in the correct formats must be included. The FMFILE may be included or not, depending on the wishes of the user. The FMFILE is used to determine values for neutron flux in units of 10^{13} neutrons/cm^2/sec (PHIFM in XDX File). The FMFILE is similar to GAMFILE in structure and is identical to it in card format. The FMFILE consists of a Z-type card followed by a single GAMANAL-type card for each sample for which PHIFM is to be determined. There may be more than one group of Z-card/GAMANAL-card pairs. The single GAMANAL card per sample can be for any nuclide. However, for that sample, the nuclide mass in micrograms must be entered on the XDX card for the sample (FMMS, Cols. 52-60 of XDX card).

Whether or not to use the FMFILE for determining the neutron flux factor is up to the NADAC user. In general, we have used multi-element standards for flux determination and have determined flux factors from a separate NADAC run on groups of such standards. The advantage of this approach is that flux factors are better determined by using multiple elements than by using a single element. The FMFILE can be used to advantage if, in the sample to be analyzed for other elements, the micrograms of a particular element is known.

The GAMANAL data for the known element can be used to make an internal flux determination for the sample rather than interpolating between flux values obtained from external standards.

We will now describe the computations and data manipulations that are performed by NADAC using the input files described above.

NADAC Computations

This description of the computations carried out by NADAC considers the mathematical basis for the computation and gives a stepwise description of the computation sequence.

MATHEMATICAL BASIS

When an irradiated sample is counted, the observed disintegration rate of a particular nuclide depends on a number of parameters: the flux and energy distribution of neutrons; nuclear cross sections; disintegration constants; irradiation, cooling, and counting times; and the amount of element in the sample. The mathematical relationships between the disintegration rate and these parameters are the basis for all non-trivial computations carried out by NADAC. The relationships presented below are for the most complex cases that can occur, namely, multiple irradiations, independent parent and daughter production, and a long counting time compared to the half-life of the decaying radionuclide.

Rate of Nuclide Production During Irradiation

In a reactor, the neutron flux consists of three components: thermal neutrons, epithermal neutrons, and "high-energy" neutrons. The rate of nuclide production by (n, γ) or (n, f) reactions depends on thermal and epithermal fluxes. The rate of production by (n, p) or (n, α) reactions depends on the high-energy flux.

The rate of production by (n, γ) or (n, f) reaction is given by:

$$R = 3.614 \times 10^{6} \left[\left(\Phi_{TH} \times \sigma_{TH} \right) + \left(\Phi_{EPI} \times RI \right) \right] \frac{W\ G}{M} , \qquad (1)$$

where:

R = production rate of (n, γ) or (n, f) product in atoms/min.

$3.614 \times 10^{6} = 60 \times 10^{-19} \times$ Avogadro's number.

Φ_{TH} = thermal flux in units of 10^{13} neutrons/cm^2/sec.

Φ_{EPI} = epithermal flux in units of 10^{13} neutrons/cm^2/sec.

σ_{TH} = thermal-neutron cross section in barns.

RI = epithermal-neutron cross section in barns.

G = isotopic abundance of target nuclide in percent.

M = atomic weight of target element in grams.

w = mass of target element in micrograms.

We define:

$$R_o = 3.614 \times 10^6 \left[\sigma_{TH} + \left(\frac{\Phi_{EPI}}{\Phi_{TH}} \right) RI \right] G/M \quad \left(\frac{\text{atoms}}{(\text{min})(\mu\text{g})} \right), \tag{2}$$

so that:

$$R = R_o \, (\Phi_{TH}) \, w \, . \tag{3}$$

The parameter R_o is a function of constants except for the ratio Φ_{EPI}/Φ_{TH}, which varies with the location within the reactor. However, within a particular location, the ratio remains reasonably constant, and thus R_o can be treated as a constant for that location. Values of R_o for the individual nuclides are stored in NUCLIB as the parameter RATE. Three versions of NUCLIB, corresponding to the three reactor regions used, are maintained. The version used by NADAC in a given analysis must be selected according to the region in which the irradiation occurred. NUCLIB library generation for given ratios of the epithermal to thermal flux can be accomplished by an auxiliary program NUCGEN which is described later.

Tables of the constants σ_{TH} and RI are given by R. Sher[2] and H. Albinson[3] in the IAEA Handbook on Nuclear Activation Cross Sections. Additional data that post-date the IAEA compilation are given by G. Gleason.[4] Approximate Φ_{EPI}/Φ_{TH} values for three regions of the Livermore Pool Type Reactor are S-2 = 0.020, E-1 = 0.041, Slow Rabbit = 0.049.

The rate of production by (n, p) or (n, α) reaction is given by:

$$R = 3.614 \times 10^6 \, (\Phi_{HIGH}) \, (\sigma_{n,p}) \, \frac{w \, G}{M} \, . \tag{4}$$

We define:

$$R_1 = 3.614 \times 10^6 \left(\frac{\Phi_{HIGH}}{\Phi_{TH}}\right)\left(\sigma_{n,p}\right)\frac{G}{M}\ , \tag{5}$$

so that:

$$R = R_1\ (\Phi_{TH})\ w\ . \tag{6}$$

Experimentally determined values of R_1 for nuclides produced by (n, p) reactions (e.g., $^{58}Ni(n,p)\ ^{58}Co$) are stored as RATE in the appropriate NUCLIB versions.

Nuclide Production by Radioactive Growth and Decay

A particular radionuclide may be produced both by decay of a radioactive parent and directly by neutron capture. This commonly occurs where both a ground state and a metastable isomer are formed during irradiation. The equations used to determine the relationship between the observed disintegration rate and the amount of element present in the sample are:

Parent $$\frac{dN_P}{dt} = R_P - \lambda_P N_P\ , \tag{7}$$

Daughter $$\frac{dN_D}{dt} = f\lambda_P N_P - \lambda_D N_D\ , \tag{8}$$

Independent $$\frac{dN_D^1}{dt} = R_D - \lambda_D N_D^1\ , \tag{9}$$

where:

N_P = no. of atoms of parent nuclide.
N_D = no. of atoms of daughter nuclide produced by decay.
N_D^1 = no. of atoms of independently produced daughter nuclide.
R_P = parent production rate (atoms/min).
R_D = independent production rate of daughter (atoms/min).
λ_P = decay constant of parent (min^{-1})(= ln 2/TPAR).
λ_D = decay constant of daughter (min^{-1})(= ln 2/TDAU).
f = fraction of parent decays leading to formation of daughter.

The relationship needed is the solution to these equations for a generalized set of irradiation, cooling, and counting times. The times involved are illustrated in Fig. 6.

In the diagram, three irradiation periods τ_1, τ_2, and τ_3 are indicated. Zero time (TZERO) is set to equal the time of completion of the final irradiation, and cooling and counting times are as shown. To simplify writing solutions to the equations, we introduce the following notation:

$$F(a,b,x) = (1 - e^{-ax})e^{-bx} , \tag{10}$$

$$\alpha_i = F(\tau_3, \delta_3, \lambda_i) + F(\tau_2, \delta_2, \lambda_i) + F(\tau_i, 0, \lambda_i) , \tag{11}$$

$$\rho_i = F(c, y, \lambda_i)/\lambda_i c , \tag{12}$$

where i = P or D.

$$K_1 = \frac{T_P}{T_P - T_D} + \frac{T_P}{T_D} , \tag{13}$$

$$K_2 = 1 - \frac{T_P}{T_P - T_D} , \tag{14}$$

where T_P and T_D are half-lives of parent and daughter, respectively; DPM = disintegration of daughter owing to parental decay, and DPM^1 = disintegration of daughter owing to independent yield.

The solutions to equations (7) through (9) are:

$$DPM = fR_P(K_1\alpha_P\beta_P + K_2\alpha_D\beta_D) \text{ (via parent)} , \tag{15}$$

$$DPM^1 = R_D\alpha_D\beta_D \text{ (direct production)} . \tag{16}$$

The gamma detector measures the sum (DPMTOT) of these two disintegration rates:

$$DPMTOT = DPM + DPM^1 , \tag{17}$$

$$DPMTOT = fR_P\left[K_1\alpha_P\beta_P + \left(K_2 + \frac{R_D}{fR_P}\right)\alpha_D\beta_D\right] . \tag{18}$$

Based on Eqs. (2) and (3) above, the values of R_D and R_P are:

$$R_D = 3.614 \times 10^6 \frac{G}{M}\left[1 + \left(\frac{\Phi_{EPI}}{\Phi_{THD}}\right)\left(\frac{RI_D}{\sigma_{THD}}\right)\right]\sigma_{THD}\, w\, \Phi_{TH} , \tag{19}$$

$$fR_P = 3.614 \times 10^6 \frac{G}{M}\left[1 + \left(\frac{\Phi_{EPI}}{\Phi_{TH}}\right)\left(\frac{RI_P}{\sigma_{THP}}\right)\right] f\sigma_{THP}\, w\, \Phi_{TH} . \tag{20}$$

When the parent exists in a metastable state and the daughter in a ground state of the same isotope, as is the case for independent daughter production, then:

$$\frac{RI_D}{\sigma_{THD}} = \frac{RI_P}{\sigma_{THP}} . \tag{21}$$

Therefore, the ratio R_D/fR_P in Eq. (18) may be expressed:

$$R_D/fR_P = \frac{\sigma_{THD}}{f\sigma_{THP}} . \tag{22}$$

Because the right side is made up of nuclear constants, the ratio R_D/fR_P is a constant. We include this constant in the NUCLIB parameter KDAU, which is defined:

$$KDAU = K_2 + \frac{\sigma_{THD}}{f\sigma_{THP}} = 1 - \frac{T_P}{T_P - T_D} + \frac{\sigma_{THD}}{f\sigma_{THP}} . \tag{23}$$

In the same notation, KPAR of the NUCLIB tables is:

$$KPAR = K_1 = \frac{T_P}{T_P - T_D} + \frac{T_P}{T_D} . \tag{24}$$

The time dependence of the basic equation can now be described by a separate function F(t), which is defined by:

$$F(t) = KPAR(\alpha_P\ \beta_P) + KDAU(\alpha_D\ \beta_D) . \tag{25}$$

The form of F(t) used here is an exact expression, which differs from the form usually given in that it provides a correct treatment of the decay

even when the counting interval c is much greater than the half-life of the nuclide counted. The term T_P/T_D in Eq. (24) does not appear in the conventional solution, and the function β_i defined in Eq. (12) is usually given as $\exp[-\lambda_i(y + c/2)]$ rather than in the correct form used here. A derivation of F(t) is given in the Appendix.

We can now write:

$$DPMTOT = fR_P \cdot F(t) = fR_{oP}\, \Phi_{TH}\, w \cdot F(t) \ , \tag{26}$$

which is a general solution for the most complex case. In this case, the value stored in NUCLIB for RATE is fR_{oP}. Computations for all other cases are also based on this general solution. For the simpler alternative cases, the values stored in NUCLIB for TPAR, TDAU, KPAR, KDAU, and RATE are adjusted to give the correct solution. Thus, where daughter is counted but has no independent production, $\sigma_{THD} = 0$. Hence:

$$KDAU = 1 - \frac{T_P}{T_P - T_D} \ . \tag{27}$$

If the nuclide counted is directly produced during irradiation, then the values stored in NUCLIB are as follows:

$$\begin{aligned} &TPAR = 1.0 \text{ (dummy parameter).} \\ &TDAU = \text{half-life of nuclide produced.} \\ &RATE = R_o \text{ for nuclide produced.} \\ &KPAR = 0.0. \\ &KDAU = 1.0. \end{aligned} \tag{28}$$

These parameters produce the correct determination of DPM per microgram when the nuclide that is counted results from direct, independent production.

Applications of Basic Equation

Most nuclides, produced by both short and long irradiations, are either directly produced or have parents whose half-lives are sufficiently short that the parent and daughter decay relationships can be omitted. The factor f, the fraction of parental decays leading to the daughter state, only applies to the few cases in which parent and daughter decay must be considered. In the following discussion, the factor f will not be specified; however, in the

construction of NUCLIB, it must be included where appropriate. The subscript P or D for the rate constant is also dropped in what follows, with the understanding that the appropriate parent or daughter production rate is used as the RATE parameter in NUCLIB. With these simplifications, the basic equation, Eq. (26), that relates disintegration rate to experimental parameters, can be expressed as follows:

$$\frac{DPMTOT}{F(t)} = R_o \, \Phi_{TH} \, w \, . \tag{29}$$

Any of the three parameters on the right can be determined if the remaining two are known. Thus, if the isotope production rate R_o and the element weight w (micrograms) are known, the thermal flux Φ_{TH} can be calculated:

$$\Phi_{TH} = \frac{DPMTOT}{F(t) \cdot R_o \, w} \, . \tag{30}$$

In our use of NADAC, a standard version of NUCLIB determines Φ_{TH} for each element in the standard. In this version of NUCLIB, the stored RATE parameter is actually the product R_o w for each nuclide of each element in the standard. The output values of NADAC then consist of a set of Φ_{TH} values, which can be averaged to obtain a best value for Φ_{TH}.

In the analysis of unknown samples, Eq. (29) is solved for w, which is the total micrograms of element in the sample [UGTOT]:

$$UGTOT = \frac{DPMTOT}{F(t) \cdot R_o \, \Phi_{TH}} \, . \tag{31}$$

The RATE value in NUCLIB is R_o, the production rate of the nuclide. The Φ_{TH} value used is based on the analysis of a standard or flux monitor. Finally, NADAC can be used to determine R_o values when micrograms of element and thermal flux are both known:

$$R_o = \frac{DPMTOT}{F(t) \cdot \Phi_{TH} \, w} \, . \tag{32}$$

In this case, the stored RATE parameter can be simply 1.0, with the factor w entered in the XDX file as sample mass.

Correction for Interfering Reactions

We will consider two types of interferences, (n, p) and (n, f). The nuclide ^{27}Mg is produced both by (n, γ) reaction on ^{26}Mg and by (n, p) reaction on ^{27}Al. The total disintegration rate observed for ^{27}Mg is the sum of these two processes:

$$DPMTOT(Mg^{27}) = \left[R_o(Mg^{26})\ \Phi_{TH}\cdot F(t)\cdot w(Mg)\right] + \left[R_1(Al^{27})\ \Phi_{TH}\cdot F(t)\cdot w(Al)\right] . \quad (33)$$

We want to determine w(Mg), the net micrograms of Mg in the sample:

$$w(Mg) = \left[\frac{DPMTOT(Mg^{27})}{R_o(Mg^{26})\ \Phi_{TH}\cdot F(t)}\right] - \left[\frac{R_1(Al^{27})}{R_o(Mg^{26})}\right] w(Al) . \quad (34)$$

The (n, p) production rate R_1, defined in Eq. (5) above, is determined for each reactor region by irradiating Al in that region. The ratio $R_1(Al^{27})/R_o(Mg^{26})$ is stored in Cols. 41-50 of NUCLIB as the parameter FTR. The total correction is computed by NADAC by multiplying this ratio by the weight (micrograms) of aluminum after TOTUG has been computed for each element present. If Al is found, a Mg correction is made. The nuclide code for the interference-producing element is stored in Cols. 71-76 of NUCLIB.

In samples where the Si:Al ratio is high, the Mg results will be incorrect, because ^{28}Al is formed both by (n, γ) on ^{27}Al and by (n, p) reaction on ^{28}Si. Therefore, the micrograms of Al used in Eq. (34) is high, the correction for Al (n, p) interference in the Mg determination is overstated, and the Mg result is low. NADAC has a built-in provision for modifying the Mg correction to allow for the Si contribution to the Al assay. However, this provision requires an expanded version of NUCLIB, which is described under the discussion of the auxiliary program NUCGEN.

The second kind of interference reaction is the fission of ^{235}U by thermal and epithermal neutrons. The nuclide ^{95}Zr is produced both by fission of ^{235}U and by (n, γ) on ^{94}Zr:

$$DPM(FISS) = R_o(FISS)\ \Phi_{TH}\cdot F(t)\cdot w(U)\ FY(^{95}Zr) , \quad (35)$$

where $FY(^{95}Zr)$ is the thermal fission yield of ^{95}Zr.

$$DPM(n,\gamma) = R_o(n,\gamma)\ \Phi_{TH} \cdot F(t) \cdot w(Zr)\ . \tag{36}$$

The observed disintegration rate for ^{95}Zr is the sum of these two reactions, so the total micrograms of Zr is:

$$UGTOT(Zr) \equiv w(Zr) = \left[\frac{DPMTOT\ (^{95}Zr)}{R_o(n,\gamma)\ \Phi_{TH} \cdot F(t)}\right] - \left[\frac{R_o(FISS)\ FY(^{95}Zr)}{R_o(n,\gamma)}\right] w(U)\ . \tag{37}$$

The ratio $R_o(FISS) \cdot FY(^{95}Zr)/R_o(n,\gamma)$ is stored in Cols. 41-50 of NUCLIB, as are the (n,p)-interference ratio data. Also, the nuclide code for the interference-producing element is stored in Cols. 71-76 of NUCLIB. For short irradiations, ^{239}U (92239) is the uranium (n,γ) product; for long irradiations, ^{239}Np (93239), the daughter of ^{239}U, is the uranium (n,γ) product.

In the foregoing treatment, the time-dependent term F(t) was the same for both the (n,γ) product and the (n,p) or (n,f) product. Where F(t) is not the same, the situation is more complex and an approximate solution is used. Consider the nuclide ^{140}La, which has a 40-hour half-life and is produced directly by (n,γ) on ^{139}La. When ^{140}La is produced by fission, it is the daughter of 12.8-day ^{140}Ba. The function F(t) for these two cases must be used in its explicit form:

$$DPM(FISS) = R_o(FISS)\ \Phi_{TH}\ w(U)\ FY(^{140}Ba)\ (KPAR\alpha_P\beta_P + KDAU\alpha_D\beta_D)\ , \tag{38}$$

$$DPM(n,\gamma) = R_o(n,\gamma)\ \Phi_{TH}\ w(La)\ \alpha_D\beta_D\ . \tag{39}$$

Because DPMTOT is the sum of the fission and (n,γ) DPM values, we have:

$$UGTOT(La) = \left[\frac{DPMTOT(^{140}La)}{R_o(n,\gamma)\ \Phi_{TH}\ \alpha_D\beta_D}\right] - \left[\frac{R_o(FISS)\ FY(^{140}Ba)\ w(U)\ \left(KPAR\ \frac{\alpha P\beta P}{\alpha D\beta D} + KDAU\right)}{R_o(n,\gamma)}\right]. \tag{40}$$

The interference-blank correction term, which appears on the right side of Eq. (40), has such a strong time dependence that at 3 days it amounts to

0.046 w(U) while at 15 days it is 3.76 w(U). To get around this problem, we treat ^{140}La and ^{140}Ba as independent nuclides in the library of gamma spectra used by GAMANAL. We assume the fission-produced ^{140}La is in transient equilibrium with ^{140}Ba. Therefore, if the latter is found by GAMANAL, a correction is made to the observed total DPM for ^{140}La. To make this correction, the final time-dependent term on the right side of Eq. (40) is replaced by the transient equilibrium ratio, TPAR/(TPAR-TDAU). In addition, both ^{140}La and ^{140}Ba are carried in NUCLIB as being independently produced, and both are assigned the half-life of ^{140}La. This approximation produces a valid correction at late times; at early times, the correction is close to the true value except when the U:La ratio in the sample is large.

Obviously, if the functional form of the time dependence of the interference is known, a version of NADAC could be written that would calculate such corrections exactly rather than by approximation. This is not done, because when multiple counts are made on an irradiated sample, the accuracy of the counts for different nuclides varies depending on the time of measurement. For example, ^{95}Zr with a 65-day half-life may not be found at all on a 3-day count but will be determined at 15 days. On the other hand, ^{239}Np, which has a 2.35-day half-life and is produced by (n,γ) on ^{238}U followed by β decay, may be easily determined at 3 days but missed at 15 days. If we wish to correct the ^{95}Zr value for the uranium fission contribution, we must first combine the elemental abundance data produced by the individual counts before making the correction. Once the combining step is carried out, time information is no longer applicable. When more than one count is made following irradiation, the values for the uncorrected total micrograms for each nuclide, determined from separate counts, are combined and a weighted mean is calculated.

Weighted Mean Calculations

In all weighted-mean calculations in NADAC and in the follow-on program MERGE, the weighting factors are set equal to the inverse square of the standard deviation. Thus, where a series of measurements x_i, each with a standard deviation s_i, are averaged to produce a weighted mean $\langle x \rangle$ and a standard deviation of the mean $\langle s \rangle$, the following equations are used:

$$\langle x \rangle = \frac{\sum_1 (x_i/s_i^2)}{\sum_1 (1/s_i^2)}, \qquad (41)$$

$$\langle s \rangle = \sqrt{1/\Sigma_i (1/s_i^2)} \tag{42}$$

For other than weighted-mean calculations, we combine the standard deviations (absolute or fractional, depending on whether additive or multiplicative processes are involved). NADAC computes the standard deviations stepwise as the calculation proceeds (see following).

COMPUTATION SEQUENCE

A condensed version of the flow diagram for NADAC computations is shown in Fig. 8, and a summary of the major steps in the computation sequence is given below.

Z-CARD Subroutine

There must be at least one Z-card, which gives irradiation time data, included in the NADAC run. If a flux monitor file is used, the first card must be a Z-card. If no flux monitor file is used or if the irradiation history of the sample differs from that of the flux monitor (e.g., the sample, but not the flux monitor, was previously irradiated), the first card of the GAMFILE must be a Z-card. Each group of GAMANAL cards that correspond to samples irradiated under different conditions must be headed by a Z-card. Whenever NADAC reads a Z-card, it branches to a subroutine that converts all time data to decimal days and resets zero time. For each nuclide listed in NUCLIB, it calculates APAR and ADAU, which are used in subsequent F(t) computations (see Eqs. (11) and (23) to (25):

$$\text{APAR} = \text{KPAR}\alpha_P \ , \tag{43}$$

$$\text{ADAU} = \text{KDAU}\alpha_D \ . \tag{44}$$

If an entry appears in Cols. 16-23 of the Z-card, the RATE and FTR values of NUCLIB will also be recomputed (see NUCGEN AUXILIARY PROGRAM). The program then returns to read the next flux monitor of the GAMANAL card and proceeds with the calculation.

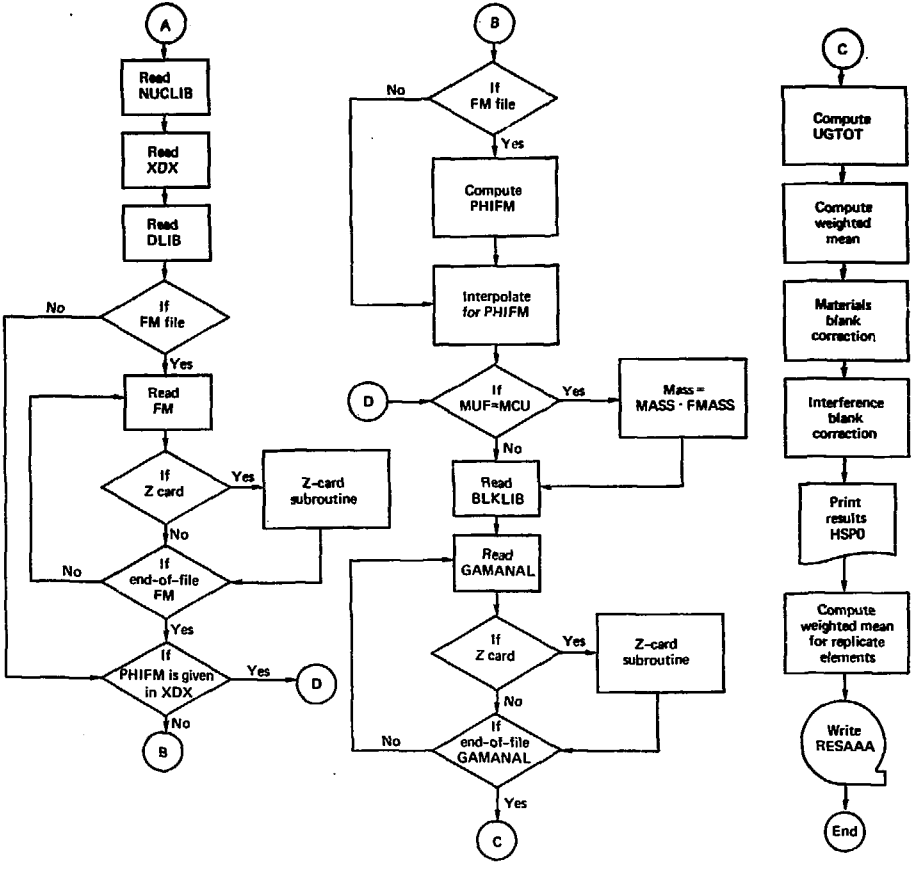

Fig. 8. Flow diagram for NADAC computations.

Flux Factor (PHIFM) Determination

Every sample listed in the XDX (cross-index) file must be assigned a flux factor value (PHIFM), which is simply the thermal neutron flux expressed in units of 10^{13} neutrons/cm^2/sec. The assignment for each sample is made according to the following order of precedence:

1. If PHIFM is entered on XDX card, it is used.
2. If there is a flux monitor file, then, for each sample having both a flux monitor card in the file and a flux monitor pass (FMMS) in the XDX file, PHIFM is computed using Eq. (30).
3. If some of the samples in the XDX file do not have PHIFM values assigned according to 1. or 2. above, these remaining samples are assigned PHIFM values by interpolation as follows:
   a. Samples that are listed between samples having PHIFM values are assigned PHIFM values based on linear interpolation.
   b. Samples that are listed externally to the first or last sample having a PHIFM value are assigned the same PHIFM value as that listed for the respective first or last sample.
4. When none of the samples in the XDX file have PHIFM values assigned according to 1. or 2. above, all samples are assigned a PHIFM of 1.0.

There is also provision for assigning a percent standard deviation (PSXFM) to each value of PHIFM. PXSFM may be entered directly on the XDX card or read as percent standard deviation from the flux monitor card (Cols. 17-20). Missing values are assigned by interpolation. When no PXSFM values are assigned, the value for all samples is set equal to zero.

Calculation of Total Micrograms

This calculation is based on the information supplied by GAMFILE. When a Z-card is encountered, the Z-card subroutine is used to reset zero time and the irradiation-dependent parameters. Each GAMANAL card is read in sequence. If the nuclide identified on the GAMANAL card is also in the NUCLIB file, the total micrograms of element is calculated according to Eq. (31). Nuclides not listed in the NUCLIB file are skipped. The quantities from Eq. (31) that are needed to calculate total micrograms (UGTOT) are: the observed disintegration rate (DPMTOT) for the nuclide from the GAMANAL card; the rate of formation

(R_o) of the nuclide, which is stored in NUCLIB as RATE; and Φ_{TH}, which is stored in the XDX array as PHIFM for the sample. The function F(t) is evaluated for each nuclide according to Eq. (25). In that equation, the quantities KPARα_P and KDAUα_D were calculated and stored as part of the Z-card subroutine. The quantities β_P and β_D are calculated by Eqs. (12) and (10):

$$\beta_i = \frac{(1 - e^{-\lambda_i c}) e^{-\lambda_i y}}{\lambda_i c} , \tag{45}$$

where:

$$\lambda_P = \ln 2/TPAR , \tag{46}$$

$$\lambda_D = \ln 2/TDAU , \tag{47}$$

$$c = T_2/86400 , \tag{48}$$

$$y = TST + 10^{-6}T_1 - TZERO . \tag{49}$$

In the expression for y, which is the cooling time, TZERO is stored as part of the Z-card subroutine, and TST and T_1 are both read directly from the GAMANAL card. Recall that the calculation of F(t) is the same for all nuclides whether a true parent-daughter relationship exists or not. When the nuclide is not a daughter but is directly produced, the parameters KPAR and KDAU of Eq. (25) are set equal to 0 and 1, respectively, so that F(t) for the directly produced nuclide is correctly calculated.

The standard deviation of the value for total micrograms for each element is calculated as follows:

$$SDUGTOT = \frac{UGTOT}{100} \times PSD ,$$

where PSD, the percent standard deviation of the disintegration rate, is read from Cols. 17-20 of the GAMANAL card. This value is used in the following calculation.

Calculation of Weighted Mean of Total Micrograms

Once the value for the total micrograms of each nuclide in each sample has been calculated, it only remains to organize the data and perform simple arithmetic. Each sample may have been counted several times. Therefore, some nuclides in a sample may have been determined by more than one count. Each count results in a calculated value for total micrograms. The initial problem is to determine a best value from the several measurements. This is done by finding the weighted mean value, using the method indicated by Eqs. (41) and (42). Organizing the data involves the following: NADAC generates an array for each irradiation code in the run. In each array, one column of data corresponds to one count of a sample. The column number corresponds to the count number LNUM, given in Col. 31 of the GAMANAL card. Each row of the array corresponds to one nuclide, and each nuclide listed in NUCLIB is included. When all the calculated values for total micrograms and for their standard deviations have been stored, their weighted means are computed and stored, together with their absolute and fractional standard deviations. The arrays are closed up by eliminating listings for nuclides that were absent. The results are sent to the printer as part of an HSPO output file. If only one count was made, the printed output is skipped.

Calculation of Net Micrograms per Unit Amount of Sample

The sequence of steps used in this calculation can be described in terms of generating a series of columns in an array.

The first column is simply a listing of the nuclides found, together with the chemical symbol for the element which produced the nuclide. The second column is the weighted mean value of the total micrograms of each nuclide found. The third column is the standard deviation of the total micrograms after adjusting to include the standard deviation of the flux factor PHIFM.

The fourth column, the materials-blank correction (in micrograms) allows for the type and amount of extraneous material in the sample. The correction is obtained by combining data from the X-card of the XDX file with the data from the Blank Library on elemental abundance per unit of each material. If two materials are used, the combined total correction is recorded.

The fifth column is the standard deviation of the total correction for the blank, based on the standard deviations of the elemental abundance values per unit of material. These values are stored as fractional standard deviations in the Blank Library.

The sixth column is the correction for the interference of (n,p) or (n,f), calculated as described above. The value calculated is the last term of Eq. (34) for (n,p) or Eq. (37) for (n,f) interference. The element producing the interference is identified by nuclide number in Cols. 71-76 (NUX) of NUCLIB. The interference correction factor (FTR) is stored in Cols. 41-50 of NUCLIB. The total micrograms of the element producing the interference is stored in the second column of the array. If Mg is found, a correction for Al interference is made. If no Al is found, TOTUG of Al is taken as zero, and no interference correction is made. Because ^{28}Al has a much shorter half-life than ^{27}Mg, Al may be found only on the first count of the irradiated sample while Mg is picked up on the second or third count. For this reason, the weighted mean of the total micrograms is calculated before the interference correction is made. One restriction in determining the interference correction is that the element producing the interference must be determined on the same irradiation (short or long) as that of the element requiring the correction. Fortunately, this has not proved to be a problem. For interference by short-lived fission products, the uranium determined from the short-lived ^{239}U is used; while for long-lived fission products, the uranium determined from the ^{239}Np daughter can be used. In all cases so far, the interfering element has been found on the same irradiation.

The seventh column lists the standard deviation for the interference correction. This is determined from the interference factor (FTR) and from the standard deviation (listed in Col. 3 of the current array) of the total micrograms of interfering element.

The eighth column lists the net weight (micrograms) of element per unit of sample. This value is calculated from a ratio, the numerator being the total micrograms minus the materials-blank and interference-blank corrections and the denominator being the sample amount read from the X-card, modified when required by the DLIB card for the sample.

The ninth and tenth columns are, respectively, the absolute and the fractional standard deviations of the net micrograms per unit of sample and are derived by appropriately combining the standard deviations for the

corresponding total micrograms, materials blank, interference blank, and sample amount.

One ten-column array is generated for each irradiated sample. As these arrays are completed, they are sent to the printer as part of the HSPO output file. The HSPO file is given titles and formats and serves as a record of the analytical results. To list these results in a form suitable for subsequent calculations, a second output file is generated that appears as RESAAA in the listing of the output file. "AAA" is taken from Cols. 2-4 of the first card in the XDX files. For convenience, we will refer to this output as the RESFILE.

RESFILE Calculations

The RESFILE carries along the final results obtained in the above calculations in a form that can be used as input to a follow-on computer code. The file consists of one line per element and gives the irradiation identification code, sample identification code, element symbol, mass units code, and net micrograms per unit mass and its standard deviation. Up to this point, we have carried one data line for each nuclide found, while the RESFILE lists one line for each element found. For several elements, amounts are determined from counts on more than one nuclide. For example, the element antimony (Sb) is usually determined from both ^{122}Sb and ^{124}Sb. For calculating a weighted-mean, as described by Eqs. (41) and (42), the results are combined into a single answer for each element found. This is the only calculation carried out in generating the RESFILE.

NADAC Output Files

When NADAC is run, two output files are generated. The first, which appears as HSPO and contains intermediate as well as final analytical results complete with titles, is intended to serve as a final report on a particular analysis. The second file, which appears as RESAAA where "AAA" signifies an irradiation identification code, is in a card-file format and serves as input to a follow-on computer program (usually MERGE which is described below).

HSPO OUTPUT FILE

The HSPO output file consists of three parts. The first consists of a single-page summary of the problem that was run. An example is the summary

for the problem described under input files, which is shown in Fig. 9. The top line gives the file name of the NUCLIB version used in running the problem. The rest of the listing consists of the Z-cards used, followed by the description of the samples to which they apply. The Z-cards give the irradiation conditions according to the format described previously. The sample data, except for cooling times, are assembled from the GAMANAL and XDX files. The cooling time, which is the time between the end of irradiation and the start of the count, is the value y used in decay calculations.

The second part of the HSPO output lists, on one or more pages per sample, the total micrograms calculated from every count for each nuclide. An example of this output section is shown in Fig. 10 together with the weighted mean values calculated from these data. The column headings (1, 2, ...) is the count number. In the listing (Fig. 10), the top entry for each pair is always total micrograms, and the bottom entry is the standard deviation. The percent standard deviation of the weighted mean and the number of counts in which the nuclide was found are also given.

The third part of the HSPO file, one page per sample, gives, for each nuclide, the intermediate and final results of the computation of net micrograms per unit of sample. An example is shown in Fig. 11. In the column

NEE01

IRRADIATION CODE	SAMPLE CODE	COUNT NUMBER	COOLING TIME(DAYS)	COUNTING TIME(SEC)	SPECTRUM NUMBER	SYSTEM NUMBER
Z221 219 162537		0072003904137 000048				
221001	RCH028	1	2.993E+00	8000	222303	T3
221001	RCH028	2	1.393E+01	20000	233102	C1
221002	RCH053	1	3.091E+00	8000	222304	T3
221002	RCH053	2	1.417E+01	20000	233103	C1
221003	RCH054	1	3.188E+00	8000	222305	T3
221003	RCH054	2	1.441E+01	20000	233104	C1
221004	RCH055	1	3.284E+00	8000	222306	T3
221004	RCH055	2	1.465E+01	20000	233105	C1
Z221 219 162537		0072003885737 000048				
221005	RCH052	1	3.382E+00	8000	222307	T3
221005	RCH052	2	1.488E+01	20000	233106	C1
221006	RCH056	1	3.479E+00	8000	222308	T3
221006	RCH056	2	1.512E+01	20000	233107	C1
221007	RCH063	1	3.576E+00	8000	222309	T3
221007	RCH063	2	1.393E+01	20000	233202	Q2
221008	RCH064	1	3.673E+00	8000	222310	T3
221008	RCH064	2	1.416E+01	20000	233203	Q2
Z221 219 162537		0072003865406 000400				
221009	RCD100	1	3.771E+00	8000	222311	T3
221009	RCD100	2	1.440E+01	20000	233204	Q2
221010	RCD101	1	3.865E+00	8000	222312	T3
221010	RCD101	2	1.463E+01	20000	233205	Q2
221011	RCD102	1	3.959E+00	8000	222313	T3
221011	RCD102	2	1.486E+01	20000	233206	Q2
221012	RCD103	1	4.053E+00	8000	222314	T3
221012	RCD103	2	1.509E+01	20000	233207	Q2
Z221 219 162537		007200				
221013	HCSD44	1	1.186E+01	66569	43740	M2
221014	HCS045	1	1.186E+01	66515	43741	D3

Fig. 9. NADAC HSPO output, part 1: Irradiation and counting summary.

1 CALCULATION OF WEIGHTED MEAN OF TOTAL MICROGRAMS
SAMPLE CODE 221001 RCH028

NUCLIDE	********1	********2	WT. MEAN	PCNT SD	N
11024 NA	1.386E+03 3.465E+01	0. 0.	1.386E+03 3.465E+01	2.500E+00	1
19042 K	6.257E+02 2.617E+02	0. 0.	6.257E+02 2.617E+02	3.170E+01	1
20047 CA	0. 0.	3.461E+03 7.235E+02	3.461E+03 7.235E+02	2.090E+01	1
21046 SC	1.994E+00 1.356E-01	1.793E+00 1.793E-02	1.797E+00 1.776E-02	9.695E-01	2
24051 CR	0. 0.	5.638E+00 1.353E-01	5.638E+00 1.353E-01	2.400E+00	1
26059 FE	4.235E+03 1.148E+03	3.669E+03 4.036E+01	3.670E+03 4.034E+01	1.099E+00	2
27060 CO	0. 0.	1.695E+00 2.682E-02	1.695E+00 2.682E-02	1.700E+00	1
30065 ZN	0. 0.	2.003E+01 1.042E+00	2.003E+01 1.042E+00	5.200E+00	1
31072 GA	9.929E+00 7.149E-01	0. 0.	9.929E+00 7.149E-01	7.200E+00	1
33076 AS	5.899E+00 1.620E-01	6.102E+00 1.817E+00	5.899E+00 1.819E-01	3.083E+00	2
34075 SE	0. 0.	2.969E+00 9.205E-02	2.969E+00 9.205E-02	3.100E+00	1
37086 RB	0. 0.	6.121E+00 3.122E-01	6.121E+00 3.122E-01	5.100E+00	1
38085 SR	0. 0.	4.856E+01 7.721E+00	4.856E+01 7.721E+00	1.590E+01	1
40095 ZR	0. 0.	4.472E+01 7.602E+00	4.472E+01 7.602E+00	1.700E+01	1
42099 MO	4.866E+00 1.489E+00	5.211E+00 2.345E-01	5.203E+00 2.316E-01	4.452E+00	2
51122 SB	9.032E-01 8.129E-02	8.856E-01 2.745E-02	8.874E-01 2.601E-02	2.931E+00	2
51124 SB	0. 0.	9.351E-01 2.244E-02	9.351E-01 2.244E-02	2.400E+00	1
55134 CS	0. 0.	3.753E-01 1.576E-02	3.753E-01 1.576E-02	4.200E+00	1
56131 BA	4.207E+02	3.733E+02	3.735E+02	1.595E+00	2

Fig. 10. NADAC HSPO output, part 2: Calculation of weighted mean of total micrograms.

headings, the symbol UG is used for micrograms, SD for standard deviation, and FSD for fractional standard deviation.

RESAAA OUTPUT FILE

The RESAAA output file consists of one line for each element of a sample. Results are listed first by irradiation-identification code and second, alphabetically, by element symbol. In the listing, because the element symbols are right adjusted, the elements with one-letter symbols

1 FINAL SUMMARY REPORT

IRRADIATION	221001				
SAMPLE CODE	RCH028				
DESCRIPTION	FC03FILTER 028	04 09:40 760213			
SAMPLE AMOUNT	2.580E+00 SCF				
MOUNTING MATERIALS	1.735E+01 SQ CM	NUCLEOPORE	+ 9.500E+01 MG	POLY BAG	
NOMINAL FLUX	2.585E+13				

NUCLIDE	ELEMENT	TOTAL UG	SD	MATERIALS BLANK UG	SD	N.F OR N.P BLANK UG	SD	NET UG/ SCF	SD	FSD
11024	NA	1.386E+03	3.465E+01	5.993E+00	4.676E-01	0.	0.	5.349E+02	1.343E+01	2.511E-02
19042	K	8.257E+02	2.617E+02	4.180E-01	1.087E-01	0.	0.	3.199E+02	1.015E+02	3.172E-01
20047	CA	3.461E+03	7.235E+02	0.	0.	0.	0.	1.342E+03	2.804E+02	2.090E-01
21046	SC	1.797E+00	1.778E-02	3.499E-04	3.371E-05	0.	0.	6.962E-01	6.890E-03	9.897E-03
24051	CR	5.638E+00	1.353E-01	1.286E-01	3.368E-02	0.	0.	2.136E+00	5.405E-02	2.531E-02
26059	FE	3.670E+03	4.034E+01	1.729E+00	1.729E-01	0.	0.	1.422E+03	1.563E+01	1.100E-02
27060	CO	1.695E+00	2.882E-02	0.	0.	0.	0.	6.571E-01	1.117E-02	1.700E-02
30065	ZN	2.003E+01	1.042E+00	1.293E-01	1.680E-02	0.	0.	7.715E+00	4.038E-01	5.234E-02
31072	GA	9.929E+00	7.149E-01	0.	0.	0.	0.	3.848E+00	2.771E-01	7.200E-02
33075	AS	5.899E+00	1.819E-01	6.175E-04	2.223E-04	0.	0.	2.286E+00	7.049E-02	3.083E-02
34075	SE	2.969E+00	9.205E-02	0.	0.	0.	0.	1.151E+00	3.568E-02	3.100E-02
37085	RB	6.121E+00	3.122E-01	0.	0.	0.	0.	2.372E+00	1.210E-01	5.100E-02
38065	SR	4.856E+01	7.721E+00	0.	0.	0.	0.	1.882E+01	2.993E+00	1.590E-01
40095	ZR	4.472E+01	7.602E+00	0.	0.	1.138E+01	3.697E-01	1.292E+01	2.950E+00	2.283E-01
42099	MO	5.203E+00	2.316E-01	5.035E-03	1.410E-03	1.725E+00	5.605E-02	1.346E+00	9.237E-02	6.863E-02
51122	SB	8.874E-01	2.601E-02	5.225E-04	1.567E-04	0.	0.	3.438E-01	1.008E-02	2.933E-02
51124	SB	9.351E-01	2.244E-02	5.225E-04	1.567E-04	0.	0.	3.623E-01	8.699E-03	2.401E-02
55134	CS	3.753E-01	1.576E-02	0.	0.	0.	0.	1.455E-01	6.110E-03	4.200E-02
56131	BA	3.735E+02	5.957E+00	1.273E-02	3.182E-03	0.	0.	1.448E+02	2.309E+00	1.595E-02
56140	UF	1.692E+00	3.774E-01	0.	0.	0.	0.	6.559E-01	1.463E-01	2.230E-01
57140	LA	8.184E+00	7.797E-02	7.315E-04	1.097E-04	3.012E-02	9.789E-04	3.160E+00	3.022E-02	9.564E-03
58141	CE	1.521E+01	3.785E-01	0.	0.	5.056E-01	1.644E-02	5.699E+00	1.468E-01	2.577E-02
60147	ND	7.051E+00	3.666E-01	0.	0.	3.928E-01	1.276E-02	2.581E+00	1.422E-01	5.510E-02
62153	SM	1.080E+00	6.612E-02	1.140E-04	1.254E-05	8.398E-05	2.729E-06	4.184E-01	2.563E-02	6.125E-02
63152	EU	1.795E-01	4.667E-03	0.	0.	0.	0.	6.958E-02	1.609E-03	2.600E-02
63154	EU	6.216E-02	1.181E-02	0.	0.	0.	0.	2.409E-02	4.578E-03	1.900E-01
63452	EU	1.170E-01	5.267E-02	0.	0.	0.	0.	4.537E-02	2.042E-02	4.500E-01
65160	TB	1.301E-01	4.294E-03	0.	0.	0.	0.	5.043E-02	1.664E-03	3.300E-02
70169	YB	5.386E-01	2.155E-02	0.	0.	0.	0.	2.088E-01	8.351E-03	4.000E-02
70175	YB	4.956E-01	1.289E-02	0.	0.	0.	0.	1.921E-01	4.995E-03	2.600E-02
71177	LU	1.421E-01	4.547E-03	0.	0.	0.	0.	5.508E-02	1.763E-03	3.200E-02
72175	HF	8.649E-01	3.027E-01	0.	0.	0.	0.	3.352E-01	1.173E-01	3.500E-01
72181	HF	1.352E+00	2.975E-02	0.	0.	0.	0.	5.242E-01	1.153E-02	2.200E-02
73182	TA	3.154E-01	1.104E-02	0.	0.	0.	0.	1.223E-01	4.279E-03	3.500E-02
74187	W	1.119E+00	1.948E-01	1.235E-03	1.729E-04	0.	0.	4.334E-01	7.549E-02	1.742E-01
91233	TH	3.425E+00	4.109E-02	0.	0.	0.	0.	1.327E+00	1.593E-02	1.200E-02
93239	U	1.817E+00	8.904E-02	4.655E-04	7.448E-05	0.	0.	7.040E-01	2.268E-02	3.250E-02

Fig. 11. NADAC HSPO output, part 3: Calculation of net micrograms per unit amount of sample.

precede those having two-letter symbols. An example of the output is shown in Fig. 12. Six items are carried on each line: irradiation (or analysis) code, sample code, element symbol, mass units code, net micrograms of element per mass unit and its standard deviation. The RESFILE output is used as input to MERGE, a code which combines the results of multiple analyses on a given sample and produces a single final answer for each element based on all available information.

221001	RCH028	K12	3.199E+02	1.015E+02
221001	RCH028	U12	7.040E-01	2.288E-02
221001	RCH028	W12	4.334E-01	7.549E-02
221001	RCH028	AS12	2.286E+00	7.049E-02
221001	RCH028	BA12	1.448E+02	2.309E+00
221001	RCH028	CA12	1.342E+03	2.604E+02
221001	RCH028	CE12	6.699E+00	1.466E-01
221001	RCH028	CO12	6.571E-01	1.117E-02
221001	RCH028	CR12	2.130E+00	5.405E-02
221001	RCH028	CS12	1.455E-01	6.110E-03
221001	RCH028	EU12	6.331E-02	1.677E-03
221001	RCH028	FE12	1.422E+03	1.589E+01
221001	RCH028	GA12	3.848E+00	2.771E-01
221001	RCH028	HF12	5.224E-01	1.140E-02
221001	RCH028	LA12	3.160E+00	3.022E-02
221001	RCH028	LU12	5.503E-02	1.763E-03
221001	RCH028	MG12	1.346E+00	9.237E-02
221001	RCH028	NA12	5.349E+02	1.343E+01
221001	RCH028	ND12	2.581E+00	1.422E-01
221001	RCH028	RB12	2.372E+00	1.210E-01
221001	RCH028	SB12	3.544E-01	6.586E-03
221001	RCH028	SC12	6.962E-01	6.890E-03
221001	RCH028	SE12	1.151E+00	3.568E-02
221001	RCH028	SM12	4.184E-01	2.563E-02
221001	RCH028	SR12	1.882E+01	2.993E+00
221001	RCH028	TA12	1.223E-01	4.279E-03
221001	RCH028	TB12	5.043E-02	1.564E-03
221001	RCH028	TH12	1.327E+00	1.593E-02
221001	RCH028	UF12	6.559E-01	1.463E-01
221001	RCH028	YB12	1.965E-01	4.287E-03
221001	RCH028	ZN12	7.715E+00	4.038E-01
221001	RCH028	ZR12	1.292E+01	2.950E+00
221002	RCH053	K12	4.555E+02	2.106E+01
221002	RCH053	U12	8.442E-01	2.444E-02
221002	RCH053	W12	4.680E-01	6.995E-02
221002	RCH053	AS12	1.813E+00	1.029E-01
221002	RCH053	BA12	1.652E+02	2.636E+00
221002	RCH053	CA12	1.479E+03	3.210E+02
221002	RCH053	CE12	7.176E+00	2.298E-01
221002	RCH053	CO12	7.944E-01	1.589E-02
221002	RCH053	CR12	4.118E+00	9.684E-02
221002	RCH053	CS12	1.816E-01	7.989E-03
221002	RCH053	EU12	7.777E-02	2.132E-03
221002	RCH053	FE12	1.619E+03	2.105E+01
221002	RCH053	GA12	4.325E+00	3.244E-01
221002	RCH053	HF12	6.354E-01	1.900E-02
221002	RCH053	LA12	4.089E+00	4.489E-02
221002	RCH053	LU12	6.844E-02	1.985E-03
221002	RCH053	MG12	1.168E+00	1.419E-01
221002	RCH053	NA12	7.807E+02	3.994E+01
221002	RCH053	ND12	3.331E+00	2.074E-01
221002	RCH053	NI12	2.685E+00	9.047E-01
221002	RCH053	RB12	2.980E+00	1.609E-01
221002	RCH053	SB12	3.185E-01	8.638E-03
221002	RCH053	SC12	8.428E-01	9.989E-03
221002	RCH053	SE12	1.107E+00	4.316E-02
221002	RCH053	SM12	5.624E-01	1.493E-02
221002	RCH053	SR12	2.288E+01	3.478E+00
221002	RCH053	TA12	1.479E-01	5.178E-03
221002	RCH053	TB12	6.257E-02	2.253E-03

Fig. 12. NADAC RESFILE output.

MERGE Input Files

Figure 13 shows an overview flow chart of the MERGE program. The execute line needed to run MERGE is: MERGE DLIB RESAAA RESBBB...RESGGG/TV. There can be only as many RESFILE's as will fit on the teletype line. The DLIB file is identical to that described under NADAC input file. The order of the files must be DLIB followed by RESFILES, but file names may be varied. The total number of lines of RESFILE information is limited to 1500. The DLIB format is given under the NADAC discussion. The RESFILE card format is as follows:

Column No.	Mnemonic (Format)	Description
1	Blank	
2-7	IRX (RG)	Irradiation or analysis code.
9-14	SPL (RG)	Sample identification code.
39-40	SS (R2)	Chemical symbol of element.
41-42	MUF (I2)	Mass units code, listed in Table 1. Same as described for NADAC; XDX card of NADAC.
45-54	NETUG (E10.0)	Micrograms per unit of sample.
57-66	SDNET (E1.0.0)	Standard deviation.

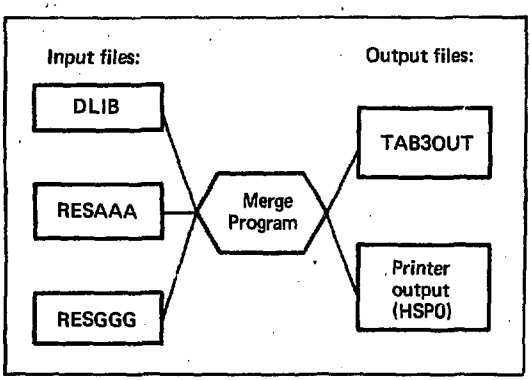

Fig. 13. Overview flow chart for MERGE.

MERGE Computations

For the most part, the MERGE code is based on sorting and searching routines. The only mathematical operation involved is the determination of weighted mean values from data sets. Equations (41) and (42) describe the mathematics.

With minor modifications, the MERGE computation resembles that described above for NADAC calculation of the weighted mean value of total micrograms. A flow diagram for MERGE computations is shown in Fig. 14. The input RESFILES are combined and sorted according to sample code, analysis (or irradiation) code, and element. For a given sample, the mass units code (MUF) must be the same for each analysis. This avoids, for example, averaging data for micrograms per stage with data for micrograms per standard cubic foot. MERGE provides for converting to new units of mass, in accordance with information provided on the DLIB card for the sample. The information that controls the change is carried in Cols. 51-70 of the DLIB card (see above DLIB Card Description). The incorporation of the mass-units conversion in MERGE was necessary, even though NADAC already would have made the change, to accommodate input RESFILES from other analysis systems, such as x-ray fluorescence or atomic absorption.

Samples whose mass codes do not match are skipped in the MERGE run. When the mass codes match, an array is generated for each sample. The rows of the array are based on the symbols of the elements arranged according to atomic number. In the columns of the array, the micrograms per unit of mass and their standard deviations are organized according to the analysis code read from the RESFILE input card. For each element, the weighted mean is calculated from the separate analyses and stored in the array along with its standard deviation. The data of the completed array make up the printed HSPO output of MERGE, which consists of one or more pages for each sample, and are ordered according to sample identification code. Appropriate titles and column headings are provided. In this printout, values of microgram per unit of mass that differ from the weighted mean values by more than three times the standard deviation are flagged by inverted arrows located below the value.

The second output file generated by MERGE is in a card-file format, consists of one card for each element of a sample, and is intended as input to subsequent data processing codes. No additional calculations are required.

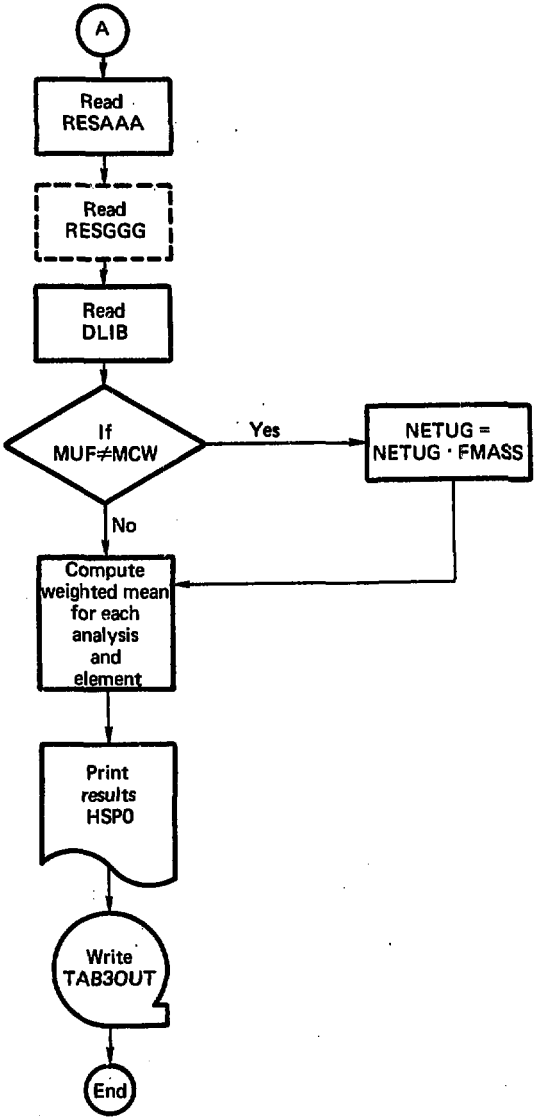

Fig. 14. Flow Diagram for MERGE computations.

Each output line consists of the sample identification code, a sample description from DLIB, the element symbol, mass units code, and the weighted mean (and its standard deviation) of the total micrograms per unit of mass. The output file appears as TAB3OUT.

MERGE Output Files

Examples of MERGE output files are shown in Figs. 15 and 16. The HSPO example shown in Fig. 15 is self explanatory. The card-format file generated as TAB3OUT (Fig. 16) lists the sample and element data. In addition, each

```
1          CONSOLIDATED ELEMENTAL ANALYSIS DATA
           SAMPLE CODE    RCH028
           DESCRIPTION    FC03FILTER    028        04 09:40 780213
           UNITS          MICROGRAMS PER             SCF

           ANALYSIS NUMBER

      221001        887001        WTD MEAN      FSD

NA  5.349E+02  5.718E+02  5.609E+02  1.302E-02
    1.343E+01  6.698E+00  7.301E+00

MG  0.         4.582E+02  4.582E+02  5.559E-01
    0.         2.547E+02  2.547E+02

AL  0.         5.947E+03  5.947E+03  3.400E-02
    0.         2.022E+02  2.022E+02

 K  3.199E+02  0.         3.199E+02  3.173E-01
    1.015E+02  0.         1.015E+02

CA  1.342E+03  1.529E+03  1.395E+03  1.698E-01
    2.804E+02  4.433E+02  2.370E+02

SC  6.982E-01  0.         6.982E-01  9.697E-03
    6.890E-03  0.         6.890E-03

TI  0.         3.353E+02  3.353E+02  1.970E-01
    0.         6.606E+01  6.606E+01

 V  0.         6.274E+00  6.274E+00  2.441E-01
    0.         2.020E+00  2.020E+00

CR  2.136E+00  0.         2.136E+00  2.530E-02
    5.405E-02  0.         5.405E-02

MN  0.         1.666E+01  1.666E+01  1.144E-02
    0.         2.134E-01  2.134E-01

FE  1.422E+03  0.         1.422E+03  1.099E-02
    1.563E+01  0.         1.563E+01

CO  6.571E-01  0.         6.571E-01  1.700E-02
    1.117E-02  0.         1.117E-02

ZN  7.715E+00  0.         7.715E+00  5.234E-02
    4.038E-01  0.         4.038E-01

GA  3.848E+00  0.         3.848E+00  7.201E-02
    2.771E-01  0.         2.771E-01

AS  2.286E+00  0.         2.286E+00  3.084E-02
    7.049E-02  0.         7.049E-02

SE  1.151E+00  0.         1.151E+00  3.100E-02
    3.566E-02  0.         3.566E-02

RB  2.372E+00  0.         2.372E+00  5.101E-02
    1.210E-01  0.         1.210E-01
```

Fig. 15. MERGE HSPO output.

028	04	09:40	760213	5.609E+02	7.301E+00	NA	12	R77/01/12
028	04	09:40	760213	4.582E+02	2.547E+02	MG	12	R77/01/12
028	04	09:40	760213	5.947E+03	2.022E+02	AL	12	R77/01/12
028	04	09:40	760213	3.199E+02	1.015E+02	K	12	R77/01/12
028	04	09:40	760213	1.395E+03	2.370E+02	CA	12	R77/01/12
028	04	09:40	760213	6.962E-01	6.890E-03	SC	12	R77/01/12
028	04	09:40	760213	3.353E+02	6.606E+01	TI	12	R77/01/12
028	04	09:40	760213	8.274E+00	2.020E+00	V	12	R77/01/12
028	04	09:40	760213	2.136E+00	5.405E-02	CR	12	R77/01/12
028	04	09:40	760213	1.866E+01	2.134E-01	MN	12	R77/01/12
028	04	09:40	760213	1.422E+03	1.563E+01	FE	12	R77/01/12
028	04	09:40	760213	5.571E-01	1.117E-02	CO	12	R77/01/12
028	04	09:40	760213	7.715E+00	4.038E-02	ZN	12	R77/01/12
028	04	09:40	760213	3.648E+00	2.771E-01	GA	12	R77/01/12
028	04	09:40	760213	2.286E+00	7.049E-02	AS	12	R77/01/12
028	04	09:40	760213	1.151E+00	3.560E-02	SE	12	R77/01/12
028	04	09:40	760213	2.372E+00	1.210E-01	RB	12	R77/01/12
028	04	09:40	760213	2.054E+01	2.450E+00	SR	12	R77/01/12
028	04	09:40	760213	1.292E+01	2.950E+00	ZR	12	R77/01/12
028	04	09:40	760213	1.346E+00	9.237E-02	MO	12	R77/01/12
028	04	09:40	760213	2.015E-02	3.019E-03	IN	12	R77/01/12
028	04	09:40	760213	3.544E-01	6.586E-03	SB	12	R77/01/12
028	04	09:40	760213	1.455E-01	5.110E-03	CS	12	R77/01/12
028	04	09:40	760213	1.369E+02	1.581E+00	BA	12	R77/01/12
028	04	09:40	760213	3.160E+00	3.022E-02	LA	12	R77/01/12
028	04	09:40	760213	5.699E+00	1.468E-01	CE	12	R77/01/12
028	04	09:40	760213	2.581E+00	1.422E-01	ND	12	R77/01/12
028	04	09:40	760213	4.276E-01	2.398E-02	SM	12	R77/01/12
028	04	09:40	760213	6.510E-02	1.532E-03	EU	12	R77/01/12
028	04	09:40	760213	5.043E-02	1.664E-03	TB	12	R77/01/12
028	04	09:40	760213	3.787E-01	1.072E-02	DY	12	R77/01/12
028	04	09:40	760213	1.865E-01	4.287E-03	YB	12	R77/01/12
028	04	09:40	760213	5.509E-02	1.763E-03	LU	12	R77/01/12
028	04	09:40	760213	5.224E-01	1.140E-02	HF	12	R77/01/12
028	04	09:40	760213	1.223E-01	4.279E-03	TA	12	R77/01/12
028	04	09:40	760213	4.334E-01	7.549E-02	W	12	R77/01/12
028	04	09:40	760213	1.327E+00	1.593E-02	TH	12	R77/01/12
028	04	09:40	760213	7.112E-01	1.995E-02	U	12	R77/01/12
028	04	09:40	760213	6.559E-01	1.463E-01	UF	12	R77/01/12
052	01A	08:54	760219	4.616E+00	2.224E-01	NA	12	R77/01/12
052	01A	08:54	760219	1.549E+01	7.717E+00	MG	12	R77/01/12
052	01A	08:54	760219	2.344E+01	1.641E+00	AL	12	R77/01/12
052	01A	08:54	760219	7.277E-01	5.015E-01	CL	12	R77/01/12
052	01A	08:54	760219	1.154E+00	4.282E-01	K	12	R77/01/12
052	01A	08:54	760219	5.521E+01	5.175E+00	CA	12	R77/01/12
052	01A	08:54	760219	2.759E-03	7.409E-05	SC	12	R77/01/12
052	01A	08:54	760219	1.734E+00	6.674E-01	TI	12	R77/01/12
052	01A	08:54	760219	3.715E-01	2.601E-02	V	12	R77/01/12
052	01A	08:54	760219	6.681E-01	1.895E-02	CR	12	R77/01/12
052	01A	08:54	760219	8.779E-01	1.014E-02	MN	12	R77/01/12
052	01A	08:54	760219	1.112E+01	4.297E-01	FE	12	R77/01/12
052	01A	08:54	760219	7.289E-03	5.394E-04	CO	12	R77/01/12
052	01A	08:54	760219	3.132E-01	2.841E-02	ZN	12	R77/01/12
052	01A	08:54	760219	9.611E-02	4.902E-03	GA	12	R77/01/12
052	01A	08:54	760219	2.795E-01	5.854E-03	AS	12	R77/01/12
052	01A	08:54	760219	6.682E-01	8.795E-03	SE	12	R77/01/12
052	01A	08:54	760219	2.262E-02	1.201E-03	BR	12	R77/01/12
052	01A	08:54	760219	9.927E-01	2.284E-01	SR	12	R77/01/12
052	01A	08:54	760219	1.039E-01	5.832E-03	MO	12	R77/01/12
052	01A	08:54	760219	5.757E-04	9.788E-05	IN	12	R77/01/12

Fig. 16. MERGE "TAB3OUT" file output.

line shows the date of the MERGE run and names the computer used for the run. This permits us to identify updates of the MERGE output. Often analyses come in at a later time and require a MERGE rerun to incorporate the later data. In our handling of this output file, the TAB3OUT label is routinely changed to a "FIN---" label. The three dashes can be used to associate the file with a particular irradiation or set of samples. FIN is an abbreviation for final.

The FINFILE format is controlled by MERGE. In terms of a card image, the format used is as follows:

Column No.	Format	Description
1-6	R6	Sample description code.
7-43	3A10,A7	Sample description obtained from Cols. 9-45 of DLIB card.
44-53	E10.0	Micrograms of element per unit of mass (Negative numbers may occur when an applied blank correction exceeds the total micrograms found.)
54-63	E10.0	Standard deviation.
65-66	R2	Chemical symbol of element. (The symbol UF indicates uranium measured by n, fission in neutron activation.)
68-69	I2	Mass units code (see Table 1).
72	-	Computer identification code.
73-80	-	Date of MERGE run.

Auxiliary Programs

In this section, we describe two programs (NUCGEN and BLKGEN) which generate libraries used by NADAC.

NUCGEN

As implied by the title, NUCGEN generates the nuclear data library NUCLIB. Most of NUCLIB is based on invariant nuclear parameters such as radioactive decay constants and thermal cross section ratios. However, the two variables RATE and FTR, which appear in NUCLIB for each nuclide, can be expressed as functions of the epithermal to thermal flux ratio. NUCGEN provides for the recomputation of RATE and FTR values if given a value for the flux ratio.

NUCGEN was written to be used as an auxiliary routine to generate a specific version of NUCLIB for a given reactor region whose flux ratio is known. However, NUCGEN is also included internally in NADAC as part of the Z-card subroutine. In the latter application, the stored parameters RATE and FTR are recomputed whenever the ratio of the epithermal to thermal flux is given in Cols. 17 to 22 of the Z-card as a five-place decimal fraction

(e.g., 0.03590). As an auxiliary program, the execute line is simply, NUCGEN NUCLIB 0.03590/T.V, where the quantity 0.03590 is the desired flux ratio. In this case, the output file appears as N03590 and is the same as the input NUCLIB except for the quantities RATE and FTR, which are recalculated for the flux ratio.

NUCGEN Input File Description

In both the auxiliary program and the Z-card subroutine applications, NUCLIB is expanded to 120 columns in width. The first 76 columns are identical to those described above under NUCLIB Card Description. The remaining columns are as follows:

Column No.	Mnemonic (Format)	Description
77-85	ROTH (E9.3)	Rate of (n,γ) or (n,p) production by thermal neutrons.
86-94	ROEPI (E9.3)	Rate of (n,γ) or (n,p) production by epithermal neutrons.
95-104	R1TH (E10.3)	Rate of (n,p) or (n,f) interference reaction for thermal neutrons.
105-114	R1EPI (E10.3)	Rate of (n,p) or (n,f) interference reaction for epithermal neutrons.
116-120	NUR (R5)	Nuclide code (ZZAAA) of element producing NUXJ by (n,p) or (n,f) reaction.

NUCGEN Computations

In Eq. (2), the stored (n,γ) RATE parameter R_o was defined. It is apparent that R_o can be expressed as the sum of two terms that reflect the thermal and epithermal (n,γ)-production rates.

$$R_o = \text{ROTHERM} + \left(\frac{\Phi_{EPI}}{\Phi_{TH}}\right) \text{ROEPI} , \tag{50}$$

where:

$$\text{ROTHERM} = \frac{3.614 \times 10^6 \, G}{M} \sigma_{TH} , \tag{51}$$

and

$$ROEPI = \frac{3.614 \times 10^6 \, G}{M} \, RI \, . \tag{52}$$

In the foregoing, where the variables are as defined for Eq. (2), the quantities G, M, σ_{TH}, and RI are constants, but the ratio Φ_{EPI}/Φ_{TH} varies significantly with position within a given reactor. When the flux ratio is known for a particular reactor region or is measured during a particular irradiation, Eq. (50) can be used to determine values of R_o for the individual nuclides.

While the above treatment of the (n,γ)- and (n,f)-reaction processes is rigorous, the analogous treatment of the (n,p) or (n,α) reactions is approximate. These latter reactions also have characteristic rates (R_1) that vary from region to region within the reactor. As indicated in Eq. (5), these reaction rates can be considered to depend on a high-energy flux, Φ_{High}, as well as on an (n,p) or (n,α) cross section. For convenience in describing the variation in R_1 with reactor position we make the assumption that the magnitude of the high-energy flux can be expressed as composed of two parts, one proportional to the magnitude of the thermal flux and the other, to the epithermal flux,

$$\Phi_{HIGH} = a \, \Phi_{TH} + b \, \Phi_{EPI} \, , \tag{53}$$

Eq. (5) can be rewritten

$$R_1 = \frac{3.614 \times 10^6 \, G}{M} \left[(a \, \sigma_{n,p}) + \left(b \, \frac{\Phi_{EPI}}{\Phi_{TH}} \, \sigma_{n,p} \right) \right] \, . \tag{54}$$

While the parameters a and b have no physical basis, they can be evaluated by measuring R_1 in reactor regions having differing epithermal to thermal flux ratios. When this is done, a reasonable linearity exists over the range of flux ratios of interest (0.018 — 0.050), and values for $(a \times \sigma_{n,p})$ and $(b \times \sigma_{n,p})$ can be set. These are used by NUCGEN to calculate R_1 values for various irradiation positions in a manner completely analogous to that used for R_o calculations.

$$R_1 = \text{R1THERM} + \left(\frac{\Phi_{EPI}}{\Phi_{TH}}\right) \text{R1EPI} \ , \tag{55}$$

where,

$$\text{R1THERM} = \frac{3.614 \times 10^6 \ G}{M} \ a \ \sigma_{n,p} \ , \tag{56}$$

$$\text{R1EPI} = \frac{3.614 \times 10^6 \ G}{M} \ b \ \sigma_{n,p} \ . \tag{57}$$

Where R_1 is the production rate of a nuclide that is used to measure the abundance of an unknown, e.g., measurement of nickel by (n,p) on ^{58}Ni, R1THERM and R1EPI are stored in the same columns of the expanded version as the ROTHERM and ROEPI. If the production rate is that of a nuclide that interferes with an (n,γ) measurement, R1THERM and R1EPI are stored as indicated above under NUCGEN input file description. In this case, the stored values are used to calculate an interference-correction factor, FTR, see Eq. (34).

$$FTR_i = (R_1)_i/(R_o)_i \ , \tag{58}$$

where the subscript i denotes the nuclide formed. To illustrate the application of the FTR_i values, we will consider ^{27}Mg which is formed by two reactions: $^{26}Mg(n,\gamma)^{27}Mg$ and $^{27}Al(n,p)^{27}Mg$. ^{27}Al is also produced by two reactions: $^{27}Al(n,\gamma)^{28}Al$ and $^{28}Si(n,p)^{28}Al$. Thus, if ^{27}Mg is nuclide i and ^{28}Al is nuclide j,

$$FTR_i = \frac{R_o[^{27}Al(n,p)^{27}Mg]}{R_1[^{26}Mg(n,\gamma)^{27}Mg]} \ , \tag{59}$$

$$FTR_j = \frac{R_o[^{28}Si(n,p)^{28}Al]}{R_1[^{27}Al(n,\gamma)^{28}Al]} \ . \tag{60}$$

NUCGEN determines the FTR factors from the calculated values of R_o and R_1 and stores them in NUCLIB as FTR values. When the 120-column expanded version of NUCLIB is used with NADAC, there is a provision for identifying cases, such as those described above, where the interfering element (e.g., Al) is itself subject to an interference reaction by another element (e.g., Si). Although

Eq. (34) is correct as it stands, it can also be expressed in terms of the subscripts defined above:

$$w_i = \frac{DPMTOT_j}{(R_o)_i \Phi_{TH} F(t)} - FTR_i w_j \ ; \tag{61}$$

however,

$$w_j = \frac{DPMTOT_j}{(R_o)_i \Phi_{TH} \cdot F(t)} - FTR_j w_k \ , \tag{62}$$

where subscript k indicates silicon. NADAC correctly handles this case when the three elements are identified as NUC, NUXJ, and NUXK in NUCLIB.

$$w_i = UGTOT_i - FTR_i[UGTOT_j - FTR_j \cdot UGTOT_k] \ , \tag{63}$$

where,

$$UGTOT_i = \frac{DPMTOT_i}{(R_o)_i \Phi_{TH} \cdot F(t)} \ , \tag{64}$$

as in Eq. (31). Thus, the expanded version of NUCLIB can be used with NADAC to identify and calculate complex interferences and also to adjust RATE and FTR values for changing epithermal to thermal flux ratios for different samples. In the latter case, however, it is necessary to list the thermal and epithermal rate constants in the supplemental part of NUCLIB (Cols. 77-120). The 80-column version of NUCLIB can be used if desired, but the two features described herein would not be available.

BLKGEN

BLKGEN is used to generate materials-blank libraries in the form required by NADAC. The execute line is: BLKGEN NUCLIB DATAFILE/TV.

The NUCLIB is the same as that used by NADAC, and the DATAFILE is a set of the card-format output files produced by MERGE as TAB3OUT. The DATAFILE may include data for up to ten blank materials. The order in which these appear in DATAFILE determines the identification code numbers (01 to 10) that are assigned to the materials blanks.

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YDB/gw/vt

Appendix. Derivation of Radioactive Growth and Decay Relationship F(t)

We define the following variables:

N_P = number of atoms of parent nuclide.

N_D = number of daughter atoms produced by parent decay.

N_D^1 = number of daughter atoms produced directly by (n,α)

R_P = parent production rate, atoms/min.

R_D = direct production rate of daughter, atoms/min.

λ_P = $\ln 2/T_P$ = disintegration rate constant for parent.

λ_D = $\ln 2/T_D$ = disintegration rate constant for daughter.

T_P, T_D = half-lives of parent and daughter, respectively.

τ = irradiation interval.

y = cooling time from end of irradiation to start of count.

c = counting interval.

f = fraction of parent decays leading to daughter.

The equations that relate the number of atoms present after irradiating for time τ and cooling for time t are as follows:

$$N_P(t) = \frac{R_P}{\lambda_P}\left[1 - e^{-\lambda_P \tau}\right]e^{-\lambda_P t}, \tag{A.1}$$

$$N_D(t) = \frac{fR_P}{\lambda_D}\left[\frac{T_P}{T_P - T_D}\left(1 - e^{-\lambda_P \tau}\right)e^{-\lambda_P t} + \left(1 - \frac{T_P}{T_P - T_D}\right)\left(1 - e^{-\lambda_D \tau}\right)e^{-\lambda_D t}\right] \tag{A.2}$$

$$N_D^1(t) = \frac{R_D}{\lambda_D}\left(1 - e^{-\lambda_D \tau}\right)e^{-\lambda_D t}. \tag{A.3}$$

If counting interval c is long relative to the half-life of the nuclide counted, the measured disintegration rate is not simply related to the true disintegration rate, which decreases exponentially during the counting interval. However, the product of the counting time and the measured

disintegration rate actually represents the number of atoms that decay during the counting interval. Thus, if we use A_P, A_D, and A_D^1 to indicate the measured disintegration rates of parent, daughter, and directly-produced radionuclides, respectively, then

$$c\,A_P = N_P(y) - N_P(y + c)\ , \tag{A.4}$$

$$c\,A_D^1 = N_D^1(y) - N_D^1(y + c)\ , \tag{A.5}$$

$$c\,A_D = \left[N_D(y) - N_D(y + c)\right] + \left[N_P(y) - N_P(y + c)\right]\ . \tag{A.6}$$

If the nuclide is directly produced, then, as in Eqs. (A.4) and (A.5), the number of disintegrations equals the number of atoms present at the beginning of the count, N(y), minus the number present at the end, N(y + c). For a daughter nuclide, the number of disintegrations equals the sum of this difference and the number of parent atoms that decayed during the same interval (Eq. (A.6)).

The observed disintegration rate of the daughter nuclide (DPMTOT) equals the sum $A_D^1 + A_D$, so that,

$$\text{DPMTOT} = \frac{N_D^1(y) + N_D(y) - N_D^1(y+c) - N_D(y+c) + N_P(y) - N_P(y+c)}{c} \tag{A.7}$$

Substituting y and y + c for t in Eqs. (A.1) to (A.3), performing the indicated operations of Eq. (A.7), and collecting terms leads to the following equation for DPMTOT:

$$\text{DPMTOT} = \frac{fR_P}{c\lambda_D}\left[\left(\frac{T_P}{T_P - T_D} + \frac{T_P}{T_D}\right)\left(1 - e^{-\lambda_P T}\right)\left(1 - e^{-\lambda_P c}\right)e^{-\lambda_P y} + \left(1 - \frac{T_P}{T_P - T_D} + \frac{R_D}{fR_P}\right)\left(1 - e^{-\lambda_D T}\right)\left(1 - e^{-\lambda_D c}\right)e^{-\lambda_D y}\right]\ , \tag{A.8}$$

which is the relationship used by NADAC.