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EVXS: A Code to Generate Multigroup Cross Sections From the Los Alamos Master Data File

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EVXS: A CODE TO GENERATE MULTIGROUP CROSS SECTIONS FROM THE LOS ALAMOS MASTER DATA FILE

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ABSTRACT

EVXS is a program for computing multigroup microscopic neutron cross sections from experimental data. It is a translation into FORTRAN-IV of a MADCAP code written by Roger Lazarus of LASL for the MANIAC computer. The sources of data contained in the library processed by EVXS are varied, but the evaluations come primarily from AWRE, LLL, and LASL. The neutron cross sections, fluxes, and secondary energy and angular distributions are given in the library in tabular form with interpolation schemes such that the integrations over neutron energies may be performed exactly in arriving at the group-averaged cross sections. Higher order components of the multigroup cross-section matrices through L = 8 have been generated using EVXS. The code is written in standard ASA FORTRAN and is designed to be computer independent. In addition to the printed results, the output can, at the user's option, include punched cards or magnetic tape suitable for input to neutronics and burn codes.

I. INTRODUCTION

For some time the Los Alamos Scientific Laboratory (LASL) has maintained a nuclear data library, referred to here as the Los Alamos Master Data File (LAMDF), consisting of a collection of sets of evaluated data prepared primarily at the Atomic Weapons Research Establishment (AWRE), Lawrence Livermore Laboratory (LLL), and LASL. The maintenance of the LAMDF and the generation of multigroup cross sections and transfer matrices from this library have been carried out at LASL using codes written by Roger Lazarus in the MADCAP language for the MANIAC computer. To make the LAMDF and the processing codes more easily available to a wider group of users and to avoid dependence on the MANIAC, the library has been transferred to the CDC-6600 computing machine, and the data handling and processing codes have been rewritten into FORTRAN-IV. Such codes are used either for the preparation and maintenance of the pointwise data on the library or for the processing of the pointwise data on the library into complete cross-section sets suitable for input to neutronics or burn codes. The EVXS program described in this report is of the latter type; it is a translation by Margaret Asprey from MADCAP into FORTRAN-IV of the original data processor for the LAMDF.

The basic function of any multigroup averaging code like EVXS is to calculate the average cross section

$$\sigma = \frac{\int dE\sigma(E)\omega(E)}{\int dE\ \omega(E)} \quad , \tag{1}$$

where integration extends over the appropriate energy interval.* The quantity $\sigma(E)$ is the cross section being averaged and $\omega(E)$ is some appropriate weighting function. In Eq. (1) and throughout this report

*All energies throughout are given and used in million electron volts; cross sections are in barns.

we follow the convention that a quantity with argument E represents the magnitude of that quantity at a particular energy E, whereas the quantity without an argument denotes an averaged value. One unique feature of the LAMDF is the inclusion not only of the pointwise neutron cross-section data, denoted generically as $\sigma(E)$ in Eq. (1), but also of the energy group structure information. The boundaries of the energy regions over which the averaging is to be performed are given and an appropriate neutron flux is tabulated at certain energy points within each of the energy groups. The flux distributions $\phi(E)$, which are normalized within each of the G energy groups, are used as the weighting functions in Eq. (1). Denoting one of the G energy groups by g and the upper and lower energy boundaries of the gth group as E_g^+ and E_g^-, the statement on normalization implies that

$$\int_g dE\ \phi(E) = 1 \quad , \tag{2}$$

where $\int_g d\Gamma$ implies $\int_{E_g^-}^{E_g^+} dE$.

Thus, Eq. (1) can be written

$$\sigma_g = \int_g dE\sigma(E)\phi(E) \quad . \tag{3}$$

Group-averaged cross sections must be calculated for each of the R reactions for which pointwise cross sections are tabulated for a given material. Denoting one of the R reactions by r, we can write, starting from Eq. (3),

$$\sigma_{r,g} = \int_g dE\ \sigma_r(E)\phi(E) \quad . \tag{4}$$

In the case of reactions for which angular probability distributions are tabulated, the nth Legendre component of the scattering cross section for the rth reaction is defined as

$$\sigma_{r,n,g} = \int_g dE\sigma_r(E)\phi(E) \int_{-1}^{+1} d\mu\ T(\mu,E)\ P_n(\mu_L) \quad , \tag{5}$$

where P_n is the Legendre polynomial of order n, μ_L is the cosine of the scattering angle in the laboratory system, $T(\mu,E)$ is the normalized angular probability distribution, and μ is the scattering angle cosine in whichever system $T(\mu,E)$ is specified. If μ is in the center-of-mass system, then μ_L is computed as a function of μ as explained in Sec. III.

Contributions to the nth Legendre component of the multigroup transfer matrices from elastic, discrete inelastic, and nonelastic scattering are calculated from certain scattering integrals which define the number of neutrons in group g that are downscattered in energy to group g´. For elastic scattering (r = 1 in the LAMDF),

$$\sigma_{l,n,g,g'} = \int_g dE\sigma_l(E)\phi(E) \int_{\Delta\mu(E,g')} d\mu T(\mu,E)P_n(\mu_L) \quad , \tag{6}$$

where $\Delta\mu(E,g')$ is the range of scattering cosine μ for which the scattered neutron has energy E´ within the boundaries of energy group g´. Note that

$$\sigma_{l,n,g} = \sum_{g'=1}^{g} \sigma_{l,n,g,g'} \quad . \tag{7}$$

For discrete inelastic scattering $\sigma_{r,n,g,g'}$ is calculated as shown in Eq. (6) except that $T(\mu,E)$ in the center-of-mass system is assumed to be 0.5. For nonelastic reactions, except fission, the contribution to the scattering matrix is defined as

$$\sigma_{r,n,g,g'} = \int_g dE\sigma_r(E)\phi(E)N_{r,g'}(E) \times \int_{-1}^{+1} d\mu_L T_r(\mu_L,E)P_n(\mu_L) \quad . \tag{8}$$

It is explicitly indicated in Eq. (8) that for nonelastic reactions $T_r(\mu_L,E)$ is always given in the laboratory system. The extra factor $N_{r,g'}(E)$ in

Eq. (8), compared with Eq. (5), is the fractional number of neutrons entering group g′ from reaction r induced by a neutron of energy E. The factor is obtained by integrating the secondary energy probability distribution $p_r(E \to E')$ over the g′ = 1, ..., g energy groups; viz.,

$$N_{r,g'}(E) = \int_{g'} dE' \, p_r(E \to E') \quad . \tag{9}$$

There are several representations, or "laws," for the secondary energy probability distributions; the same parametrization of these laws is used in the LAMDF as is used in the UKAEA Nuclear Data Library.[1]

For fission reactions, the fission spectrum χ, the average number of neutrons per fission $\bar{\nu}$, and the total fission cross section are calculated. For example:

$$(\nu\sigma_f)_g = \int_g dE \, \bar{\nu}(E) \, \sigma_f(E) \, \phi(E) \quad , \tag{10}$$

where $\bar{\nu}(E)$ is the average number of neutrons per fission produced at energy E.

The formats and conventions used for describing the pointwise neutron cross-section data in the LAMDF are similar to those of the UKAEA Nuclear Data Library.[1] There are, however, enough significant differences to warrant a complete description of the LAMDF in Sec. II. The types of neutron cross-section data stored and the way they are used in calculation are also discussed in Sec. II, and details of the format for the library are presented there, along with a description of the materials in the library at this writing. The methods of calculation are described in detail in Sec. III, and in Sec. IV the EVXS PROGRAM is described. A user's manual for EVXS is given in Sec. V.

II. DESCRIPTION OF THE LOS ALAMOS MASTER DATA FILE

A. Library Format

1. General Remarks. The library tape that is used as input to PROGRAM EVXS contains energy group structure information and many sets of evaluated cross sections. The division of the binary library tape into NS files* is shown schematically in Fig. 1. The first file contains the energy group structure information and the remaining NS-1 files contain the neutron cross-section data for NS-1 materials, one material per file. The first record of File 1 has descriptive information to identify the edition of the LAMDF and the total number of files, NS, on the library tape. The remaining NG records in File 1 contain the energy boundaries and neutron fluxes for each of the NG group structures. As indicated in Fig. 1, the general structure of all remaining files, one for each material, is the same. The first record contains the material identification number and other control parameters; the next R records contain cross sections for the R reactions appropriate for this material, as well as information about the energy distribution of secondary neutrons; the final ND records contain the angular distribution information.

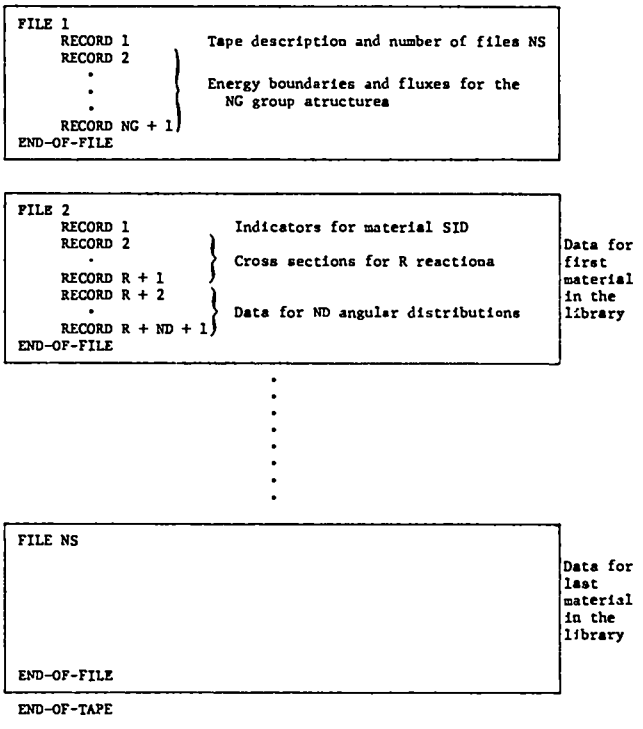

Fig. 1. Overall file structure of library tape.

*Our use of the word file conforms with the general practice of the computer industry; the NS files on the library tape are well defined binary files separated by END-OF-FILE marks which can be detected using "IF (EOF)" tests. NS, NG, ND, KG, etc., are single integers in the FORTRAN sense.

2. Group Structures. A detailed description of the first file of the binary library tape is given in Table I. The integer variables can take on values no larger than those indicated in parentheses following the variable name; the size of the descriptive arrays TAD and GDES as provided in PROGRAM EVXS is given in the parentheses following those variable names. For each of the NG group structures in the library there is one long record containing a unique identification number, alphanumeric descriptive information, the group boundaries E_g, the flux distributions $\emptyset(E)$, and appropriate control information. There may be as many as 80 energy groups for which a total of up to 500 values of the flux distribution can be tabulated, allowing many values within each group. The 2KG words at the end of the record contain KG pairs of values of the flux $\emptyset(E)$ and energy E. These values are alternately read into arrays PH_k and EK_k with subscript k running from 1 to KG. The first energy EK_1 corresponds to the low energy boundary of the first group g = 1; the highest energy EK_{KG} corresponds to the upper boundary of the Gth energy group. The function $\emptyset(E)$ represented by the values of PH_k is assumed to vary smoothly enough to be regarded as continuous (see Sec. II.D.1) everywhere except at the group boundaries E_g. This discontinuity is a result of the required within-group normalization, namely:

$$\int_{E_g^-}^{E_g^+} dE\ \emptyset(E) = 1 \quad , \tag{11}$$

TABLE I

CONTENTS OF LIBRARY TAPE - FILE 1

	Variable Name	Description	Format	Comments
	Record 1:			
	TAD (100)	Tape description	Display (A10)	
	NS ($\leq$ 500)	Total number of files	Integer	Positive
Group Structure Library	Record 2:			
	GID	Group set identification number	Integer	Positive
	GDES (8)	Description of group set	Display (A10)	
	G($\leq$ 80)	Number of energy groups	Integer	Positive
	MG_g, g = 1, ..., G	Two packed integers I1 and I2 to delimit range of indices in PH and EK for group g	Octal	I1 = MG(g)/2^{24} I2 = MG(g) - I1*2^{24}
	GE_g, g = 1, ..., G	Median energy for each group	Floating	
	KG($\leq$ 500)	Number of flux and energy pairs	Integer	Positive
	(PH_k,EK_k), k = 1, ..., KG	Pairs of values of the flux and energy	Floating	Energy in MeV
	Record 3: (and following)			
	{ Record 2 is repeated to End-of-File NG - 1 Times (NG $\leq$ 100) }			

where the lower and upper energy bounds of the gth group are designated E_g^- and E_g^+, respectively. Thus for every value of g except g = G, there will be some value of k such that $EK_k = EK_{k+1} = E_g^+$ which also equals the lower bound E_{g+1}^- for the next higher energy group. The array MG contains for each of the G groups two values of k, packed into one word, which indicate the lower and upper energy bounds of each group in the EK table. Each 60-bit word in MG is divided into two parts--the first 36 bits for an integer I1 and the remaining 24 for integer I2. The range of values for k corresponding to one energy group is then delimited by I1 and I2. From the discussion of the discontinuities in the tabulation of $\emptyset(E)$, it can be seen that I1 for group g + 1 is one more than I2 for group g. The GE array consists of weighted mean energies for each of the G groups in the group structure; these are used only in special calculations described in Sec. III.F.

3. Control and Cross-Section Records. As shown in Fig. 1, all remaining files on the library tape have the same structure; each file is associated with some material and is tagged with a unique identification number. Within each material file there are three different types of records. The contents of the first record are summarized in Table II. The first word in the record is the integer identification number SID. When reference is made to a particular SID in the LAMDF, it is understood that one is referring to a particular set of evaluated cross sections for some material; there can be, and often are, several different evaluations for the same material. The second word of the record gives the number of sets of angular distributions stored (for this SID) on the library tape; the following ND integers are identification numbers for these sets of which there can be no more than 25. The next 8 words contain the cross-section set description (SDES)--80 optional alphanumeric characters to identify the SID more completely as to material described and source of data. The total number of reactions for which cross sections are tabulated in succeeding records is given by the integer R. By "reaction" we mean elastic scattering, discrete inelastic scattering, nonelastic scattering, fission, and absorption as will be discussed in connection with Table V. The TIDR array consists of R integers to indicate which of the ND sets of angular distributions is appropriate for each reaction. The first set of angular distributions is always used for elastic scattering. The nonexistence of an appropriate angular distribution set among the ND sets available is indicated by a negative number in the TIDR array. Exceptions and extensions to these rules are discussed in Sec. III.

The cross sections for the R reactions are tabulated on a common energy mesh. The total number of energies NES must be less than 3000; this control parameter is followed by NES values of the energies. The IDR array contains integers to identify the type of cross section represented by each of the R reactions. These numbers are larger by 1000 than the standard reaction identification numbers summarized in Table V. The cross sections for each reaction may not be given at all of the NES energies, but only in the energy range over which they are available. For example, cross sections for a reaction with a threshold energy are not tabulated at energies below the threshold. The array ME contains R octal numbers with two packed integers, J1 and J2, one pair for each reaction. They are packed in the same manner as described in Sec. II.A.2 for the MG array. Integers J1 and J2 are indices for entries in the ES array corresponding to the initial and final energies for which the reaction cross section is tabulated. The R entries in the IRS array give the number of entries in the ESJ array for each of the R reactions; the ESJ block contains information used to describe the energy distribution of secondary neutrons. The reaction energy Q values for each of the R reactions are stored in the QR array. The last three integers in Record 1 of a material file are the proton number Z for the material, a flag to indicate whether the material is a single isotope or a mixture of more than one, and a final control flag K2 to describe the energy distributions of outcoming neutrons. The last flag, K2, is not used in PROGRAM EVXS. With the exception of the energies ES, reaction energies Q, and descriptive display information SDES, all items in the first record of a material file are control parameters in integer format used to govern the reading of succeeding records in the material file.

TABLE II

FIRST RECORD OF A MATERIAL FILE ON LIBRARY TAPE

CONTROL PARAMETERS FOR MATERIAL SID

Variable Name	Description	Format	Comments
Record 1:			
SID	Cross-section set identification number	Integer	Positive
ND($\leq$ 25)	Number of sets of angular distributions	Integer	Positive
$TIDS_n$, n = 1,..., ND	Identification numbers for angular distribution sets in order as stored on library tape	Integer	
SDES(8)	Description of cross-section set	Display (A10)	
R($\leq$ 50)	Number of reactions	Integer	Positive
$TIDR_r$, r = 1,..., R	Identification of angular distribution to be used with rth reaction	Integer	If negative, no angular distribution
NES($\leq$ 2000)	Number of energies in FS block	Integer	Positive
ES_i, i = 1,..., NES	Energies at which cross sections are tabulated	Floating	
IDR_r, r = 1,..., R	Reaction identification numbers	Integer	Positive
ME_r, r = 1,..., R	Two packed integers, J1 and J2, to indicate range of entries in ES for which reaction r cross sections are tabulated	Octal	$J1 = ME(r)/2^{24}$ $J2 = ME(r) - J1*2^{24}$
IRS_r, r = 1,..., R	Number of words in ESJ for the rth reaction	Integer	Positive numbers greater by 1000 than the identification numbers in Table V
QR_r, r = 1,..., R	Energy released by rth reaction	Floating	
NZ	Z number for material	Integer	Positive
MIX	Nonzero for isotope mixture	Integer	Positive
K2	Number of data to describe energy distribution of outcoming neutrons	Integer	Positive; not used in EVXS

The contents of the R records following the first record are summarized in Table III. For each reaction there is one record consisting of the cross sections SIG and the secondary energy parameters ESJ. The number of cross-section values for the rth reaction is calculated from the two packed integers J1 and J2 in ME_r; the number of ESJ values for reaction r is given by IRS_r. Data will be given in the ESJ block for all reaction types that produce secondary neutrons unless the secondary energy distributions can be implicitly determined from the angular distribution information. Thus, for elastic scattering (r = 1 in the LAMDF) and discrete inelastic scattering, the ESJ block is omitted. There should be entries in ESJ for all reactions r such that $15 \leq IDR_r \leq 31$, which are the nonelastic reactions including inelastic scattering to the continuum, fission, (n,2n), and (n,3n).

4. Angular Distribution Records. The contents of the last ND records of a material file for a particular SID are summarized in Table IV. As shown in Fig. 1 and indicated in the table, the first of these records in the material file is numbered R + 2. The first word of each of the ND records is the number TID used to identify the set of angular distributions; this word is followed by eight words of alphanumeric descriptive information TDES.

The set of angular distributions consists of NED normalized probability distributions $T(\mu,E_i)$ at NED energies E_i. The integer SYS indicates whether the probabilities are given in the center-of-mass or laboratory system; the atomic mass A of the material is measured in units such that for the ground state of C^{12}, A is exactly 12. The specifications for the probability distributions $T(\mu,E_i)$ are given in the TK block which has a total of KT entries, where KT must be no larger than 3000. For each of the NED energies, there is a group of entries in the TK array; the MD array contains NED octal numbers consisting of two integers K1 and K2 packed as described for the MG block in Sec. II.A.2. These specify the first and last entries in the TK array for each of the NED energies. The number of entries in TK for the ith energy is K = K2 - K1 + 1. The probability functions are given either in tabular form or in terms of Legendre expansion coefficients. Integer flag LEGN specifies the number of energies for which probability distributions are given in terms of Legendre coefficients. If LEGN = 0, the probabilities are tabulated for all energies and the TK block contains K/2 pairs of values for μ and $T(\mu,E_i)$ for each of the energies with the pairs in order of increasing μ, with $\mu = -1$ and $\mu = +1$ always present. If LEGN > 0, then for all energies E_i such that $i \leq$ LEGN, the TK block contains Legendre expansion coefficients F_n. The number of coefficients is specified by NF, the first word of the TK block for this energy; this is followed immediately by the NF values of F_n. It is evident that NF = K - 1. When LEGN > 0 and i > LEGN, the TK block contains $(\mu,T(\mu,E_i))$ pairs as described for LEGN = 0. The integer NINC specifies the number of intervals to be used in the numerical integration with respect to μ over the range $-1 \leq \mu \leq +1$.

Angular distributions for elastic scattering are given in the center-of-mass system; for discrete inelastic reactions, isotropic scattering in the center-of-mass system is assumed; for nonelastic reactions the laboratory system is used. In any case where this convention is not followed, PROGRAM EVXS proceeds as if it were, but a warning message is printed.

B. Reactions Available

Within the file for each material SID, cross sections are given for many different reactions. A summary of all the reactions for which reaction cross-section data can be entered in the LAMDF is listed in Table V. The various reactions are

TABLE III

CONTENTS OF LIBRARY TAPE
CROSS-SECTION RECORDS FOR MATERIAL SID

Variable Name	Description	Format	Comments
Record 2: (r = 1)			
SIG_j, j = 1,..., IS	Cross sections for the rth reaction	Floating	Where IS = J2 - J1 + 1. J1 and J2 obtained from ME_r
ESJ_i, i = 1,..., IRS_r	Parameters to be used in calculating the function $P_r(E \to E')$ (r = 2,..., R) to describe the energy distribution of secondary neutrons	Floating	Omitted if IRS_r = 0
Record 3: (r = 2)			
Same format as Record 2			
.			
.			
.			
Record R + 1: (r = R)			
Same format as Record 2			

TABLE IV

CONTENTS OF LIBRARY TAPE
ANGULAR DISTRIBUTION RECORDS FOR MATERIAL SID

Variable Name	Description	Format	Comments
Record R + 2: (n = 1)			
TID	Identification number for angular distribution set	Integer	Positive
TDES(8)	Description of angular distribution set	Display (A10)	
NED(≤ 400)	Number of energies at which distributions are given	Integer	Positive
E_i, i = 1,..., NED	Energies	Floating	Positive
SYS	1 or 2 - Center-of-mass or laboratory system	Integer	Always 1 for elastic Always 2 for nonelastic
A	Atomic mass of material	Floating	Mass of C^{12} (ground) = 12 units
LEGN(≤ NED)	Number of energies with Legendre coefficients	Integer	At present, if LEGN ≠ 0, LEGN = NED
KT(≤ 3000)	Number of words in TK	Integer	Positive
TK_k, k = 1,..., KT	Specifications for the probability distribution T(μ,E)	Floating	
MD_i, i = 1,..., NED	Two packed integers K1 and K2 to indicate range of entries in TK for the ith energy	Octal	K1 = MD(i)/2^{24} K2 = MD(i) - K1*2^{24}
NINC	Number of intervals to be used in integrating with respect to μ	Integer	Positive
Record R + 3: (n = 2)			
Same format as Record 2			
.			
.			
Record R + ND + 1: (n = ND)			
Same format as Record 2			

identified by number in accordance with the classification scheme prescribed for the UK Library,[1] the only difference being that reactions numbered 1, 3, and 4 are omitted from the LAMDF. The reactions can be grouped into broader categories: elastic, discrete inelastic, nonelastic, and absorption. For all materials, the first reaction (r = 1) is elastic scattering with ID = 2.

Inelastic scattering to the discrete levels is represented by reactions with identification numbers ID such that 5 ≤ ID ≤ 14 and 51 ≤ ID ≤ 80; ID numbers 81 through 100 have been reserved for future needs in describing discrete inelastic reactions. For discrete inelastic reactions the notation (n,n′j) is used to represent inelastic scattering such that the target nucleus is left in its jth excited state. Inelastic scattering in which sufficient energy is transferred from the incident neutron to the target to leave it with energy

TABLE V

REACTIONS FOR WHICH NEUTRON CROSS-SECTION DATA CAN BE ENTERED IN THE LAMDF

Number[a]	Type[b]	Reaction	Reaction Description	
2	1	(n,n)	Elastic (note that reactions numbered 1, 3, and 4 are omitted from the LAMDF)	
5	1	(n,n´1)	Discrete inelastic	
6	1	(n,n´2)		
7	1	(n,n´3)		
8	1	(n,n´4)		
9	1	(n,n´5)		
10	1	(n,n´6)		
11	1	(n,n´7)		
12	1	(n,n´8)		
13	1	(n,n´9)		
14	1	(n,n´10)		
15	1	(n,n´C)	(n,n´) to the continuum	Nonelastic reactions for which secondary energy distributions are described in terms of laws
16	2	(n,2n)		
17	3	(n,3n)		
18	0	(n,f)	Fission total = (n,f) + (n,n´f) + ...	
19	0	(n,f)	No prefission neutrons	
20	1	(n,X)	(X = n´f) } Not currently handled	
21	2	(n,X)	(X = 2n´f) } by EVXS	
22	1	(n,n´α)		
23	1	(n,n´3α)		
24	2	(n,2nα)		
25	3	(n,3nα)		
26	2	(n,2niso)		
27	1	(n,n´p)		
28	1	(n,n´γ)		
29	1	(n,n´d)		
30	1	(n,n´He^3)		
31	1	(n,n´t)		
32-50	0	(N,X)	Undefined (allowed for other nonelastic reactions)	
51	1	(n,n´11)	Discrete inelastic (continued)	
52	1	(n,n´12)		
53	1	(n,n´13)		
54	1	(n,n´14)		
55	1	(n,n´15)		
.	.	.		
.	.	.		
.	.	.		
78	1	(n,n´38)		
79	1	(n,n´39)		
80	1	(n,n´40)		
81-100	0	(n,X)	Undefined (allowed for other discrete inelastic reactions)	
101	0	(n,par ab)	Parasitic absorption	
102	0	(n,γ)	Absorption	
103	0	(n,p)		
104	0	(n,d)		
105	0	(n,t)		
106	0	(n,He^3)		
107	0	(n,α)		
108	0	(n,2α)		
109-150	0	(n,X)	Undefined (allowed for other absorption reactions)	

[a]The convention used for reaction identification numbers is the same as that prescribed for the UK Library.[1]

[b]The number of outcoming neutrons from the given reactions is given by TYPE.

corresponding to the continuum of levels is represented by (n,n´C), ID = 15.

Nonelastic reactions with $15 \leq ID \leq 31$ are those for which secondary neutrons are produced whose energy distributions can be described in terms of so-called laws which will be described in Sec. II.D.2. The fission reactions which have $18 \leq ID \leq 21$ are a subset of the nonelastic reactions.

Absorption reactions are those for which there are no outcoming neutrons, so that it is meaningless to speak about the energy distribution of secondary neutrons. The absorption reactions for which data can be entered in the LAMDF are listed under $101 \leq ID \leq 108$. Numbers $109 \leq ID \leq 150$ are reserved for other absorption reactions.

The integers listed under TYPE describe the number of outcoming neutrons from a reaction; however, an exception is made with the fission reactions which have TYPE = 0 and which are handled specially. The type description employed here follows the convention used in the UK format.[1]

C. Materials and Group Structures Available in the LAMDF

Although the purpose of this report is to describe a multigroup averaging code and the format of the library on which the processor operates, it is appropriate to consider the current contents of the LAMDF as a means of better understanding the type of information contained therein. The most recent edition (January 1972) contains cross sections for 78 materials, each with a separate SID; thus, as discussed in connection with Fig. 1, there are 79 files on the library tape. This number is considerably less than 500, which is the maximum number of files allowed. In Table VI there is a list of all the cross-section sets currently in the library, with the cross-section set identification number SID and the set description. The line of alphanumeric information in the column titled "Description" is a reproduction of the 80 characters of data contained in the SDES array for each SID. The integer ND for each SID is listed in the third column under the title "Number of Sets of Angular Distributions." In this edition of the library the largest value of ND is 3, much less than the allowed maximum of 25. The number of reactions R is listed in the fourth column; the largest value is 27 (maximum allowed is 50)

TABLE VI

CROSS-SECTION SETS IN THE LAMDF

SID	Description	Number of Sets of Angular Distributions	Number of Reactions	Number of Energies
11	H UK-LASL 28 JUN 1965	1	2	112
21	HE2 LASL 1966$	1	3	78
22	HE4 LASL 1965$	1	1	49
120	MO-$ JAN 65 LRL	1	4	126
151	P31 JAN 65 LRL	1	2	800
180	AR- JAN 65 LRL$	1	4	76
190	K- JAN 65 LRL$	1	5	185
251	M255 JAN 65 LRL	1	3	170
310	GA-$ JAN 65 LRL	1	4	73
411	IN93 JAN 65 LRL	1	4	102
420	MO-$ JAN 65 LRL	1	4	65
480	CD-ISL NOV 67	1	4	327
640	GD-$ JAN 65 LRL	1	3	444
922	U23% JAN 65 LRL	1	6	41
923	U235 JAN 65 LRL	1	6	148
924	U236 JAN 65 LRL	1	6	48
928	U280 JAN 65 LRL	1	6	36
942	PU239 JAN 65 LRL	1	6	82
943	PU240 JAN 65 LRL	1	6	74
951	AM242 LRL	1	6	455
2008	HE3 BEST AVAIL AT APR 65	2	2	111
2009	HE- UK NOV 65#	1	2	282
2022	BE222 BEST AVAIL AT APR 65	2	6	282
2026	F9-C BEST AVAIL AT APR 65	2	4	163
2034	O16 KAPL-UK OXYGEN 1965	1	27	653
2035	AL27 BEST AVAIL AT APR 65	2	15	390
2036	FE-# BEST AVAIL AT APR 65	2	27	783
2040	PU241 UK NOV 65	2	6	822
2045	CR-# UK MAY 66	3	20	888
2046	NI-C UK OCT 1965	3	20	699
2052	C- KAPL-UK CARBON 1969	1	4	353
2138	CA-C BEST AVAIL AT APR 65	1	3	119
2182	ZR2# BEST AVAIL AT APR 65	3	19	680
2190	TI- BEST UK AT APR 1965$	1	10	417
2214	LI6 BEST AVAIL AT APR 65	2	3	181
2225	LI7 BEST AVAIL AT APR 65	2	7	108
2222	AC227 UK OCT 65	1	15	170
2249	CU-2 UK 1967	1	15	356
2252	T UK-LASL DEC 67	2	2	78
2254	D UK-LASL DEC 67	2	3	162
3005	U238 UK JAN 69 SPECIAL	2	12	1919
3006	CL2 UK JAN 69 SPECIAL	3	6	210
3008	HE3 UK JAN 69 SPECIAL	2	5	111
3010	H UK JAN 69 SPECIAL	1	2	62
3017	CR- UK JAN 69 SPECIAL	1	4	230
3019	NI- UK JAN 69 SPECIAL	1	6	321
3036	FE56 UK JAN 69 SPECIAL	2	13	321
3105	GA- UK JAN 69 SPECIAL	1	4	160
3186	GD- UK JAN 69 SPECIAL	1	5	160
3201	PU240 UK JAN 69 SPECIAL	2	9	444
3203	PU241 UK JAN 69 SPECIAL	2	6	324
5509	BE9 BE9 LRL - JUNE 70	1	5	61
5513	H1A LASL - LRL - AUG 70	1	15	632
5514	O16 O- LRL OXYGEN APRIL 1971	1	12	155
5528	FE56 FE LRL - JUNE 70	1	5	138
5547	U235 U235 LRL - JUNE 70	1	6	203
5550	U238 U235 LRL - JUNE 70	1	6	215
5554	PU239 PU239 LRL - JUNE 70	1	7	241
5555	PU240 PU240 LRL - JUNE 70	1	6	244
5558	FE FISSION LRL MAY 70	1	4	156
5930	H LASL HYDROGEN(LS) DEC-70	1	2	156
7081	O- UK-KAPL OXYGEN 1965	2	9	399
7160	SULFUR 05R MAY 1967	1	4	602
7220	HE3 UK JANUARY 71	1	3	78
7521	S32 LRL SULPHUR JAN28 71	1	6	230
7921	U233 NOV 67 LRL	1	6	208
8050	B-$ LRL OCT 1966	1	4	87
8051	B10 LRL OCT 1966	1	3	87
8071	H1A LRL OCT 1966	1	6	87
8140	SI-$ LRL OCT 1966	1	4	171
8260	FE- LRL NOV 67	1	3	138
8731	ZA181 LRL OCT 1966	1	4	168
8740	W-$ LRL OCT 1966	1	4	91
8921	U233 NOV 67 LRL	1	6	208
8925	U237 LRL NOV 67	1	6	39
8926	U238 LRL OCT 1966	1	6	119
8927	U239 LRL NOV 67	1	6	30
8941	PU238 LRL OCT 1966	1	6	39

which occurs in the oxygen evaluation (SID = 2034) prepared in 1965 at the Knolls Atomic Power Laboratory (KAPL). The number of energies NES in the ES block for each SID is listed in the last column of Table VI. By far the largest number of energy points (NES = 1919) is required for the U-238 evaluation, SID-3005. Such a large number is not unreasonable because many points are required to describe adequately the resonance behavior of the uranium cross section. However, this number is much lower than the maximum of 3000 indicated in Table II.

The 34 group structures stored in File 1 of the most recent edition of the LAMDF are listed in Table VII. For each separate group structure there is a group set identification number GID followed by the description of the set as contained in the GDES array. The number of groups G and the number of flux, energy pairs KG are listed in the third and fourth columns of the table. The largest number of groups in any set is 68 and the largest number of energy points for which values of the flux are tabulated is 169. These numbers are well under the maximum values of 80 and 500 allowed in Table I for variables G and KG, respectively.

Additional cross-section sets and group structures can be added to the library tape at any time. The FORTRAN code XSMOD has been written at LASL by Martha Hoyt to perform these functions. It should be emphasized, however, that when using any edition of the LAMDF, one is not limited to the group structures contained therein but can instead use any arbitrary weighting structure using cards as input.

D. Additional Details About Use of the Data

1. Log-Log Interpolation Schemes. Energy-dependent quantities about which information is given in the LAMDF—quantities like the flux distributions $\phi(E)$, reaction cross sections $\sigma_r(E)$, and the average number of neutrons per fission $\nu(E)$—are assumed to vary smoothly enough with energy that the functional dependence can be represented by the coordinates of end points of linear segments taken from ln X vs ln E plots, X representing ϕ, σ_r, or ν. In the "log-log" representation the quantity X(E) for $E_k \leq E \leq E_{k+1}$ is interpolated between the tabulated pairs of values (E_k, X_k) and (E_{k+1}, X_{k+1}) using the formula

$$\ln\left[\frac{X(E)}{X_k}\right] = \ln\left[\frac{X_{k+1}}{X_k}\right] \ln\left[\frac{E}{E_k}\right] \Big/ \ln\left[\frac{E_{k+1}}{E_k}\right] \qquad (12)$$

with $E_k \leq E \leq E_{k+1}$.

Equation (12) can be rewritten

$$\ln\left[\frac{X(E)}{X_k}\right] = Y \ln\left[\frac{E}{E_k}\right] \quad , \qquad (13)$$

where

$$Y = \ln\left[\frac{X_{k+1}}{X_k}\right] \Big/ \ln\left[\frac{E_{k+1}}{E_k}\right] \quad . \qquad (14)$$

Furthermore, if we define

$$S = \ln X_k - Y \ln E_k \quad , \qquad (15)$$

then the interpolated value X(E) can be expressed

$$X(E) = e^S E^Y \quad . \qquad (16)$$

This form is extremely convenient since the integrals, such as those in Eq. (4), can then be written in the form

$$\int_{E_g^-}^{E_g^+} dE\, X_1(E)\, X_2(E) \ldots\ldots X_n(E) \quad , \qquad (17)$$

where

$$X_n(E) = e^{S_n} E^{Y_n} \quad , \qquad (18)$$

and

$$E_k \leq E_g^- \quad \text{and} \quad E_g^+ \leq E_{k+1} \quad , \qquad (19)$$

TABLE VII

GROUP STRUCTURES IN THE LAMDF

GID	Description	Number of Groups	Number of Flux, Energy Pairs
1	SPECTRAL INDEX GODIVA	1	1
6	HANSEN-SANDMEIER	6	24
10	MAR 68 10-GROUP REVERSED	10	33
15	W. CROWE 15-GROUP	15	16
16	HANSEN 16-GROUP	16	47
17	HARRIS-LABAUVE 17 GP JUN 70	17	34
18	C. MILLS 18-GROUP	18	169
19	BELL 19-GP AUG 68	19	56
21	W-4 21 GP FEB 67	21	56
25	SANDMEIER 25 -GROUP	25	57
26	SANDMEIER 26-GROUP	26	59
27	SANDMEIER 27-GROUP AUG11-70	27	61
28	ROACH 28-GROUP	28	30
30	DUDZIAK 30-GP 1/22/68	30	60
34	RJ LABAUVE 34-GROUP DEC14-70	34	68
37	7 GROUP TEST	7	14
41	REVERSED 4 GROUP	4	14
68	68 GROUPS 0.25 LETHARGY WIDTHS 0.414EV	68	136
69	C MILLS 6 GP JUN 67	6	75
102	T-2 CLYDE	10	20
108	ROACH 10-GROUP	10	38
109	W-4 10 GP FEB 67	10	38
119	R J LABAUVE 19 GROUPS 4/20/71	19	38
141	W-4 #1 APR 69	14	46
142	W-4 #2 APR 69	14	43
151	H. ISRAEL BOTTOM 15 GPS MAR 68	15	30
161	BELL-MILLS 16 GP	16	32
162	HANSEN 16-GP FLAT AUG 70	16	32
189	C. MILLS 18-GP OF JULY 67	18	99
197	W-4 U235 FISS SPEC	1	42
198	SID 3041 FISSION SPECTRUM	1	76
250	RISE 25-GROUP	25	58
301	W-4 30 GROUP 10/8/70	30	76
555	RJ LABAUVE 50-GROUP FLAT WT JAN20 71	50	100

which can be integrated exactly. Hence the integral can be further simplified to

$$e^{S_1} \cdot e^{S_2} \cdots e^{S_n} \int_{E_g^-}^{E_g^+} dE \cdot E^{Y_1} \cdot E^{Y_2} \cdots E^{Y_n} \qquad (20)$$

or

$$e^{S_1+S_2+\cdots+S_n} \int_{E_g^-}^{E_g^+} dE \cdot E^{Y_1+Y_2+\cdots+Y_n} \quad . \qquad (21)$$

The lower and upper energy bounds of the gth group are designated E_g^- and E_g^+, as described previously. Also note that because of the logarithmic interpolation, it is impossible to use values of 0.0 for either X_k or E_k. Instead, in all cases 10^{-20} is used to approximate 0.0.

2. Secondary Energy Probability Distributions. For a reaction with identification number ID such that $15 \leq ID \leq 31$, the entry in the IRS array will be nonzero and, as mentioned in connection with Table III, the cross-section record will contain values of ESJ as well as the cross sections themselves. The secondary energy probability distributions $p(E \rightarrow E')$--the probability that neutrons of energy E' will be produced by an incident neutron of energy E--are calculated from entries in ESJ.

For each reaction, $p(E \rightarrow E')$ is normalized such that

$$\int_0^{E'_{max}} p(E \rightarrow E')\, dE' = TYPE \quad , \qquad (22)$$

where E'_{max} is the maximum possible secondary neutron energy. Each probability distribution can be broken down into partial distributions $F_k(E \rightarrow E')$ such that

$$p(E \rightarrow E') = \sum_{k=1}^{10} w_k F_k (E \rightarrow E') \quad , \qquad (23)$$

where w_k is the fractional probability that the distribution $F_k(E \rightarrow E')$ is to be used to describe the outgoing neutrons. Equation (22) is obtained by requiring that

$$\sum_{k=1}^{10} w_k = TYPE \quad , \qquad (24)$$

where TYPE is the number of secondary neutrons produced in the reaction. Each $F_k(E \rightarrow E')$ is defined by a different analytic representation called a law; we say that w_k is the weight for the kth law. As indicated in Eq. (23), provision has been made for as many as 10 laws, although only 8 are now being used in the LAMDF. The distributions $F_k(E \rightarrow E')$ are analytic in secondary energy E' only; separate tabulations of the parameters and/or data for the various laws must be given for many values of the incident neutron energy E. Thus, the ESJ block is broken into sublists, one for each of several incident neutron energies E_i; each of the sublists can be broken into no more than eight sub-sublists, one for each of the eight allowable laws. All numbers in the ESJ block are in floating point form. Various combinations of negative numbers serve as flags to separate the sublists and sub-sublists within the ESJ block. All data other than these flags will be ≥ 0.0. A detailed description of the organization of the ESJ block is given in Fig. 2.

The length of the block for the rth reaction as given in the rth entry of the IRS array is determined by the particular reaction, the number of incident neutron energies E_i at which the probability distributions are to be calculated, and the number of laws required to specify each distribution. Two things are always the same: (a) The first word in the block is the identification number for the reaction in floating point. (b) The last word of the ESJ block will be -1.0. As shown in Fig. 2, the main part of the block is broken up into several sublists ending with two negative numbers -5.0, -2.0. The first word of each sublist is an incident neutron energy E_i followed by up to eight sub-sublists which correspond to the eight laws currently provided for. Each sub-sublist begins with a pair of numbers w_k and L_k, where L_k = 1.0, 2.0,..., 7.0, or 10.0 and w_k is the weight to be associated with the kth law; the sub-sublist is ended with the number -4.0. Thus there are really three negative numbers at the end

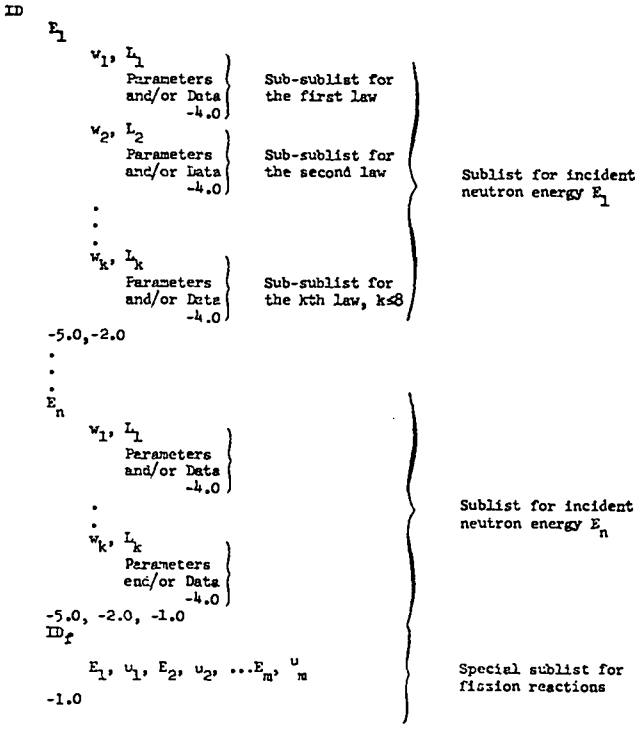

Fig. 2. Arrangement of the ESJ block.

of each sublist: the number -4.0 signifies the end of the sub-sublist for the last law and the pair -5.0, -2.0 marks the end of the sublist for some energy. The sublists are arranged so that the energies E_i appear in order of ascending magnitude. Each probability distribution $p(E \rightarrow E')$ is assumed to be independent of E over energy ranges whose boundaries are delineated by the E_i; the probability distributions are not interpolated between the energies for which the sublists are given. Instead, one assumes

$$p(E \rightarrow E') = p(E_i \rightarrow E') \qquad (25)$$

for $E_i \leq E < E_{i+1}$. At energies above E_f, the energy of the final sublist,

$$p(E \rightarrow E') = p(E_f \rightarrow E') \quad . \qquad (26)$$

The sublists are repeated until the final energy sublist which ends with four negative numbers -4.0, -5.0, -2.0, and -1.0. This combination of negative numbers marks the end of the ESJ block except in the case of the fission reactions with ID = 18, 19, 20, or 21. For fission reactions the set of four numbers is followed by a special block containing data on the energy dependence of ν, the average number of neutrons per fission. The first word of the special block is an identification number ID + 4000 in floating point; i.e., for ID = 18 the first word of the special block would be 4018.0. Then follows a sequence of pairs of values of energy and ν; this special block is terminated with the negative number -1.0.

To understand fully the ESJ array, the functional forms of the probability distributions must be described and the arrangement of the parameters thereof as read from the sub-sublists must be defined. The eight laws currently provided for in EVXS are similar to those prescribed for the UK Library.[1] The details of the laws as prescribed for the LAMDF are given here.

Law 1. In this representation the secondary neutrons are emitted with fixed discrete energies E'_i so that

$$F_1(E \rightarrow E') = \sum_{i=1}^{I} f_i \, \delta(E' - E'_i) \quad , \qquad (27)$$

where f_i is the fraction of the secondary neutrons emitted with energy E'_i and $\delta(E' - E'_i)$ is the Dirac delta-function distribution used to represent the discrete nature of energy E'_i. It is required that

$$\left| \sum_{i=1}^{I} f_i - 1.0 \right| \leq 0.005 \quad . \qquad (28)$$

The entries in the sub-sublist for this law are w_1, L = 1.0, E'_1, f_1,..., E'_I, f_I, -4.0.

Law 2. This law is used to represent secondary neutrons with discrete energies E'_i which are directly related to the incident neutron energy E. The distribution $F_2(E \rightarrow E')$ is expressed

$$F_2(E \rightarrow E') = \sum_{i=1}^{I} f_i \, \delta(E' - E'_i) \quad , \qquad (29)$$

but here

$$E_i' = A_i(E - D_i) \quad , \tag{30}$$

where E is the incident neutron energy, D_i is some discrete energy decrement, and A_i is the reduction factor. As for Law 1, the f_i sum to unity. The entries in the sub-sublist for this law are w_2, L = 2.0, D_1, A_1, f_1,..., D_I, A_I, f_I, -4.0.

Law 3. The distribution function for this law is a continuous normalized spectrum f(E') independent of the incident energy E. Thus,

$$F_3(E \to E') = f(E') \quad ; \tag{31}$$

the function f(E') is given in tabular form so that the entries in the sub-sublist for this law are w_3, L = 3.0, E_1', $f(E_1')$,..., E_I', $f(E_I')$, -4.0.

Law 4. Neutrons with secondary energy E' are represented by the normalized distribution function $F_4(E \to E')$ which is tabulated as a function of E' for several values of E. The sub-sublist for this law looks just like that for Law 3, because the dependence on E is introduced solely through the use of several sublists. Specifically, the sub-sublist for some energy E has the form w_4, L = 4.0, E_1', $f(E \to E_1')$,..., E_I', $f(E \to E_I')$, -4.0.

Law 5. The distribution function for this law is written

$$F_5(E \to E') = g(E, E'/E^q) \tag{32}$$

where q = 1/2. The function $g(E,E'/E^q) = g(E,x)$, where $x = E'/E^q$, is tabulated as a function of x so that the sub-sublist for this law for a particular energy has the form w_5, L = 5.0, x_1, $g(E,x_1)$,..., x_I, $g(E,x_I)$, -4.0.

Law 6. The distribution function for this law has the same form as that for Law 5 except that q = 1. It should be noted that Laws 4, 5, and 6 have the same form except that q = 0, 1/2, and 1, respectively.

Law 7. A detailed representation of the generalized fission spectrum is given by the distribution for this law. The probability distribution is written

$$F_7(E \to E') = \alpha \frac{E'}{T^2} e^{-\frac{E'}{T}} + (1 - \alpha) \frac{2}{\sqrt{\pi}\, B^{3/2}} \times \sqrt{E'}\, e^{-\frac{E'}{B}} \quad , \tag{33}$$

where

$$B = a + b(\bar{\nu} + 1)^{1/2} \quad , \tag{34}$$

$$T = c(E - E_f)/(14 - E_f) \text{ (energies in MeV)}, \tag{35}$$

$$E_f = \text{threshold energy for the } (n,n'f) \text{ reaction} \quad , \tag{36}$$

and

$$\alpha = \frac{\sigma_{n,n'f} + \sigma_{n,2n'f}}{\bar{\nu}(\sigma_{n,f} + \sigma_{n,n'f} + \sigma_{n,2n'f})} \quad . \tag{37}$$

Quantities a, b, c, and E_f are input through the ESJ array; the remaining quantities (the E, $\bar{\nu}$ pairs) must be obtained from the special section at the end of the ESJ array. The dependence of $F_7(E \to E')$ on the incident neutron energy E is stated explicitly in the expression for T, but it is implicit in the quantities $\bar{\nu}$, the average number of neutrons per fission, and the various fission reaction cross sections used in calculating B and α. The simple Maxwellian fission distribution

$$F_7(E \to E') = \frac{2}{\sqrt{\pi}} \frac{1}{B^{3/2}} \sqrt{E'}\, e^{-\frac{E'}{B}} \quad , \tag{38}$$

is a special case with α = b = 0.0.

This distribution is normalized so that

$$\int_0^\infty F_7(E \to E')\, dE' = 1.0 \quad . \tag{39}$$

At present EVXS is programmed to handle only the cases with α = b = 0.0. Herein lies the origin of the comment in Table V concerning reactions with

ID = 20 and 21, the (n,n´f) and (n,2n´f) reactions not currently handled by EVXS. However, provision has been made in the sub-sublist for this law to include all four input parameters; its general form is w_7, L = 7.0, a, b, c, E_f, -4.0.

Law 10. An evaporation spectrum is represented by Law 10; viz.,

$$F_{10}(E \to E') = \frac{E'}{T^2} e^{-E'/T} \quad , \tag{40}$$

where

$$T = \sqrt{E}/a \quad . \tag{41}$$

Dependence on energy E is introduced through energy dependence of parameter a. For a given E the sub-sublist for Law 10 is simply written w_{10}, L = 10.0, a, -4.0. This law is really one special limit (α = 1) of Law 7.

For the tabulation in Laws 3, 4, 5, and 6, it is assumed that linear interpolation between tabulated points is adequate to describe the functions so that the trapezoidal rule may be used in the numerical integrations carried out with respect to the secondary energy E´.

3. Angular Distribution Representations. The contents of the angular distribution records were outlined in the discussion centered around Table IV. It was pointed out that the specifications for the probability distributions $T(\mu,E_i)$, either in tabular form or in terms of Legendre coefficients, are contained in the TK array. The number of words KT contained therein cannot be explicitly defined; it depends on whether Legendre coefficients or tabulated data are given, and on the degree of anisotropy of the angular distributions. Obviously, fewer data points are required to specify an isotropic distribution than one which is highly anisotropic. There are sufficient data to specify NED normalized probability distributions $T(\mu,E_i)$ corresponding to the NED incident neutron energies E_i. The MD array contains octal numbers (packed as described in Sec. II.A.2) to specify which entries in the TK array are intended for each of the NED energies. The normalization requirement implies that

$$\int_{-1}^{+1} T(\mu,E_i)d\mu = 1.0 \quad . \tag{42}$$

It is understood that the angular distributions at intermediate energies are to be obtained by linear interpolation between those at energies E_i and E_{i+1}, regardless of whether $T(\mu,E_i)$ is tabulated directly or obtained from Legendre coefficients. Thus,

$$T(\mu,E) = T(\mu,E_i) + (E - E_i) \times \frac{T(\mu,E_{i+1}) - T(\mu,E_i)}{E_{i+1} - E_i} \quad , \tag{43}$$

where $E_i < E < E_{i+1}$. The normalization is thereby preserved at the intermediate energy E. It remains to define explicitly how the information in the TK block for each energy is to be introduced into the calculation.

Where the parameter LEGN is greater than zero, the probability distributions for the first LEGN energies are specified in terms of Legendre coefficients. In such cases the first word of the sub-block in TK contains an integer NF to specify the number of Legendre coefficients that immediately follow; specifically, the words are NF, F_1, F_2,..., F_{NF}. From these the probability distribution is calculated

$$T(\mu,E_i) = \frac{1}{2}\left\{1 + \sum_{n=1}^{N}(2n + 1)F_n P_n(\mu)\right\} \quad , \tag{44}$$

where $P_n(\mu)$ is the nth order Legendre polynomial and $N \leq NF$. The upper limit N of the summation deserves explanation.

Angular distribution data in the LAMDF may be given in terms of Legendre coefficients for nonelastic reactions only; furthermore, whether specified in terms of Legendre coefficients or tabulated functions, the probability functions $T(\mu_L,E)$ are in the laboratory system (SYS = 2) for these reactions. The expression in Eq. (8) for calculating nth order Legendre components of cross sections for such reactions contains an integral of the form

$$\int_{-1}^{+1} T(\mu_L,E)\, P_n(\mu_L)\, d\mu_L \quad , \tag{45}$$

where n = 0,..., NMAX and NMAX is the maximum order of anisotropy desired. Using the expression for $T(\mu_L,E)$ as found in Eq. (44) we can write Eq. (45) as

$$\frac{1}{2}\int_{-1}^{+1} \left\{1 + \sum_{m=1}^{N} (2m+1)F_m P_m(\mu_L)\right\} P_n(\mu_L) d\mu_L$$

$$= \delta_{o,n} + \sum_{m=1}^{N} F_m \delta_{m,n} \quad , \tag{46}$$

where $\delta_{i,j}$ is the celebrated Kroenecker delta. We have taken advantage of the orthogonality of the Legendre polynomials over the range $-1 \leq \mu_L \leq +1$ in arriving at Eq. (46). Since n will be no greater than NMAX, there is no contribution to the summation in Eq. (46) for m > NMAX. Thus it is clear that N = NMAX or NF, whichever is smaller, and that the integral in Eq. (45) can be expressed as a sum of the Legendre coefficients for the expansions of the angular distribution data.

In a set of angular distributions there are NED energies for which probability distributions $T(\mu,E)$ are given. The first LEGN thereof are specified in terms of Legendre coefficients; the remaining NED-LEGN distributions are tabulated so that each sub-block for these distributions consists of $(\mu,T(\mu,E))$ pairs starting with $\mu = -1.0$ and ending with $\mu = +1.0$.

III. METHODS OF CALCULATION

A. General Remarks

For any single material for which cross sections are tabulated in the LAMDF, group-averaged cross sections are calculated by PROGRAM EVXS, reaction by reaction. The various reactions (summarized in Table V) can be grouped into two broad categories depending on whether or not secondary neutrons are produced.

Absorption reactions are those for which there are no outcoming neutrons so that it is meaningless to speak about calculating a contribution to the scattering matrix. As indicated in Table V, these reactions with ID $\geq$ 101 and TYPE = 0 absorb neutrons and, therefore, one can calculate only a total cross section for neutron disappearance due to each such reaction.

The other category of reactions--those for which secondary neutrons are produced--is more difficult to calculate because one must average these cross sections over both the incoming and outgoing energy groups. This second category can be subdivided into two classes: (1) Those reactions for which there is a direct kinematical relationship between the outgoing energy and the scattering angle so that the width of the outgoing energy group g′ can be related to a range of the scattering cosine μ. (2) Those reactions for which the secondary energy distributions are not directly related to the scattering angle, but are described instead in terms of the fractional probability that a neutron of incident energy E will produce secondary neutrons of energy E′. Legendre components of the scattering matrix are calculated for all reactions in the second category.

For absorption reactions, only the total cross section is calculated. For elastic, discrete inelastic, and nonelastic reactions, the total and scattering cross sections are computed. For fission reactions, the total cross section, the fission fraction $\chi_{g'}$, and the average number of neutrons per fission $\bar{\nu}$ are calculated. After the multigroup, microscopic neutron cross sections have been calculated for all reactions, the total cross sections and scattering matrices are combined into DTF format suitable for input to neutron transport calculations. In Sec. III we present in detail the procedure for group-averaging the data in the LAMDF described in Sec. II.

B. Absorption

For each reaction r such that $101 \leq ID \leq 108$ and TYPE = 0, a total cross section is calculated for each of the G neutron energy groups; viz.,

$$\sigma_{r,g} = \int_{E_g^-}^{E_g^+} dE\, \phi(E)\, \sigma_r(E) \quad (g = 1, 2,..., G) \ , \tag{47}$$

where $\sigma_r(E)$ is the absorption cross section and $\phi(E)$ is the normalized weighting function. The upper and lower energy bounds of the gth group are E_g^+ and E_g^-. Note that E_g^+ is the same as E_{g+1}^-.

Both $\phi(E)$ and $\sigma_r(E)$ are tabulated as linear segments on log-log plots so that the integral in Eq. (47) can be performed exactly. The energy range E_g^- to E_g^+ is divided into I smaller intervals determined by the values of E_j and E_k at which the cross sections and fluxes, respectively, are tabulated. Equation (47) can then be written

$$\sigma_{r,g} = \sum_{i=1}^{I} \int_{El_i}^{E2_i} dE_i \, \phi(E_i) \, \sigma_r(E_i) \quad , \tag{48}$$

where the low energy boundary El_1 of the first interval is E_g^- and the high energy boundary $E2_I$ of the Ith group is E_g^+. As shown in Sec. II, the expression for the flux in any one of the intervals such that $E_k \leq E_i \leq E_{k+1}$ can be written

$$\phi(E_i) = e^{P_i} E_i^{X_i} \quad , \tag{49}$$

where

$$X_i = \frac{\ln(\phi_{k+1}/\phi_k)}{\ln(E_{k+1}/E_k)} \tag{50}$$

and

$$P_i = \ln(\phi_k) - X_i \ln(E_k) \quad . \tag{51}$$

Similarly, for $\sigma_r(E_i)$ in the range $E_j \leq E_i \leq E_{j+1}$,

$$\sigma_r(E_i) = e^{S_i} E_i^{Y_i} \quad , \tag{52}$$

where

$$Y_i = \frac{\ln(\sigma_{j+1}/\sigma_j)}{\ln(E_{j+1}/E_j)} \tag{53}$$

and

$$S_i = \ln(\sigma_j) - Y_i \ln(E_j) \quad . \tag{54}$$

Note that P_i, S_i, X_i, and Y_i are constants. Thus,

$$INT \equiv \int_{El_i}^{E2_i} dE_i \, \phi(E_i) \, \sigma_r(E_i) = \int_{El_i}^{E2_i} dE_i \, e^{P_i} E_i^{X_i} e^{S_i} E_i^{Y_i} = e^{P_i+S_i} \int_{El_i}^{E2_i} dE_i \, E_i^{X_i+Y_i} \quad . \tag{55}$$

In the case $X_i + Y_i + 1 = 0$,

$$INT = e^{P_i+S_i} [\ln(E_i)] \Big|_{El_i}^{E2_i} \quad . \tag{56}$$

When $X_i + Y_i + 1 \neq 0$,

$$INT = e^{P_i+S_i} \frac{E^{X_i+Y_i+1}}{X_i + Y_i + 1} \Big|_{El_i}^{E2_i} \quad . \tag{57}$$

The total integral is the sum of the integrals over the I smaller intervals. As we have seen, the integrals for $\sigma_{r,g}$ are performed exactly; no numerical approximations have been made. Of course, the group-averaged total cross section is no more accurate than the representation of the experimental data as found in the LAMDF.

C. Scattering Computed Using Angular Distributions

The cross sections for scattering reactions must be averaged over both incoming and outgoing energies. For elastic (ID = 2) and discrete inelastic ($5 \leq ID \leq 14$ and $51 \leq ID \leq 80$) reactions, there is one outgoing neutron for every incident neutron, and a definite relationship exists between the cosine of the scattering angle and the energy of the outgoing neutron. For these reactions we calculate Legendre components of the cross section for scattering neutrons from incident energy group g to scattered group g′, where $g' \leq g$. Upscattering in energy of the neutrons is not allowed, although it would be relatively simple to add to the code if it were needed.

The integral expression to be evaluated is

$$\sigma_{r,n,g,g'} = \int_g dE\ \phi(E)\ \sigma_r(E) \int_{\Delta\mu(E,g')} d\mu \times T(\mu,E)\ P_n(\mu_L) \quad , \tag{58}$$

where $\Delta\mu(E,g')$ is the angular range allowed for scattered neutrons having energies within the bounds of the g'th group. Here, as before, $\phi(E)$ and $\sigma_r(E)$ are the weighting flux and the cross section, μ_L is the scattering cosine in the laboratory system, $P_n(\mu_L)$ is the Legendre polynomial of order n, $T(\mu,E)$ is the angular distribution, and μ is the scattering cosine in whichever system $T(\mu,E)$ is specified. The abbreviation

$$\int_g = \int_{E_g^-}^{E_g^+}$$

has been used in Eq. (58) and will be used throughout. It is clear that for the lowest energy group ($g' = 1$), $\mu_{min} = -1.0$, and μ_{max} cannot exceed +1.0 in the highest secondary energy group $g' = g$.

The total cross section $\sigma_{r,n,g}$ for reaction r and group g is the sum of the cross sections for scattering into group g and all lower energy groups:

$$\sigma_{r,n,g} = \sum_{g'=1}^{g} \sigma_{r,n,g,g'} \quad , \tag{59}$$

which can be written

$$\sigma_{r,n,g} = \sum_{g'=1}^{g} \int_g dE\ \phi(E)\ \sigma_r(E) \int_{\mu_{min}(E,g')}^{\mu_{max}(E,g')} \times d\mu\ T(\mu,E)\ P_n(\mu_L) \quad . \tag{60}$$

The fractional number of neutrons of energy E scattered into secondary energy group g' is given by the angular distribution integral

$$N(E) = \int_{\mu_{min}(E,g')}^{\mu_{max}(E,g')} d\mu\ T(\mu,E)\ P_n(\mu_L) \quad . \tag{61}$$

In Eqs. (58), (60), and (61) the determination of the limits on μ depends on whether the scattering is elastic or discrete inelastic, and these cases must be considered separately. First let us consider some additional general details about the evaluation of the integral in Eq. (58).

The integral in energy over the gth group in Eq. (58) is computed in a fashion similar to that for the absorption reactions. The energy range E_g^- to E_g^+ is divided into smaller intervals determined by the energies at which the fluxes, cross sections, and angular distributions are tabulated. As in Eq. (48) and those following, let the flux $\phi(E)$ be expressed in the range $E_k \leq E1 \leq E \leq E2 \leq E_{k+1}$ as

$$\phi(E) = e^P\ E^X \quad ,$$

let the cross section $\sigma_r(E)$ be expressed in the range $E_j \leq E1 \leq E \leq E2 \leq E_{j+1}$ as

$$\sigma_r(E) = e^S\ E^Y \quad ,$$

and let the angular distributions $T(\mu,E)$ be given at energies E_a and E_b such that $E_a \leq E1 \leq E \leq E2 \leq E_b$. Upon substitution of the above expressions, that portion of the integral in Eq. (58) over the energy interval $E1 \leq E \leq E2$ can be written

$$INT = \int_{E1}^{E2} dE\ e^P\ E^X\ e^S\ E^Y\ N(E) \tag{62a}$$

$$= e^{P+S} \int_{E1}^{E2} dE\ E^X\ E^Y\ N(E) \tag{62b}$$

$$= e^{P+S} \int_{E1}^{E2} dE\ E^X\ E^Y\ \frac{B(E)}{E} \quad , \tag{62c}$$

where the angular integral N(E) is defined in Eq. (61). Recall that P, S, X, and Y are constants.

Equation (62c) serves to define B(E). From Eqs. (61) and (62c) we further define

$$B_0 \equiv B(E_a) = E_a \int_{\Delta\mu(E_a,g')} d\mu\ T(\mu,E_a)\ P_n(\mu_L) \qquad (63)$$

and

$$B_1 \equiv B(E_b) = E_b \int_{\Delta\mu(E_b,g')} d\mu\ T(\mu,E_b)\ P_n(\mu_L) \quad . \qquad (64)$$

The angular integrations are performed only for those energies at which the angular distributions are specified. An approximation is made in assuming that the quantity B(E) at intermediate energy E may be obtained by linear interpolation between the quantities B_0 and B_1 at energies E_a and E_b. The following explicit form for B(E) is used:

$$B(E) = \frac{B_0(E_b - E) - B_1(E_a - E)}{E_b - E_a}$$

$$(E_a \leq E \leq E_b) \quad . \qquad (65)$$

Substituting into Eq. (62c) we find that

$$INT = e^{P+S} \int_{E1}^{E2} dE\ \frac{E^{X+Y}}{E}\ \frac{B_0(E_b - E) - B_1(E_a - E)}{E_b - E_a} \quad , (66)$$

which can be written

$$INT = \left[B_1 - B_0\right] \left\{ \frac{e^{P+S}}{E_b - E_a} \int_{E1}^{E2} dE\ E^{X+Y} \right\}$$

$$+ \left[E_a * E_b \left(\frac{B_0}{E_a} - \frac{B_1}{E_b} \right) \right] \left\{ \frac{e^{P+S}}{E_b - E_a} \int_{E1}^{E2} dE\ E^{X+Y-1} \right\} \quad . \qquad (67)$$

The terms in the square and curly braces are combined in SUBROUTINE COEF; the expressions inside the curly braces are actually evaluated in SUBROUTINE SSUM. Using the notation which is essentially that of the FORTRAN programming, we let

$$PS = P + S$$

$$XY = X + Y$$

$$EE = E_b - E_a$$

$$AA = B_1 - B_0$$

$$BB = E_a * E_b \left(\frac{B_0}{E_a} - \frac{B_1}{E_b} \right)$$

$$ASUM = \frac{e^{PS}}{EE} \int_{E1}^{E2} dE\ E^{XY}$$

$$BSUM = \frac{e^{PS}}{EE} \int_{E1}^{E2} dE\ E^{XY-1} \quad . \qquad (68)$$

Then

$$INT = AA * ASUM + BB * BSUM \quad . \qquad (69)$$

Generally,

$$ASUM = \frac{e^{PS}}{EE}\ \frac{E2^{XY+1} - E1^{XY+1}}{XY + 1} \qquad (70)$$

and

$$BSUM = \frac{e^{PS}}{EE}\ \frac{E2^{XY} - E1^{XY}}{XY} \quad . \qquad (71)$$

If $|XY| < 0.001$, then the following approximations are used:

$$ASUM = \frac{e^{PS}}{EE} (E2 - E1) \qquad (72)$$

and

$$BSUM = \frac{e^{PS}}{EE} \ln\left(\frac{E2}{E1}\right) \quad . \qquad (73)$$

Furthermore, if $|XY + 1| < 0.001$, special attention is given to the evaluation of ASUM, which is re-written as

$$ASUM = \frac{e^{PS}}{EE} \int_{E1}^{E2} dE\ \frac{E^{XY+1}}{E} \quad . \qquad (74)$$

The numerator of the integrand is expanded;

$$E^{XY+1} \approx 1 + (XY + 1)\ \ell n(E) + \ldots\ldots \quad ,$$

where the first two terms of the expansion are assumed sufficient because $XY + 1 \approx 0$. Hence, ASUM is approximated as

$$ASUM = \frac{e^{PS}}{EE} \int_{E1}^{E2} dE \left[1 + (XY + 1)\ \ell n(E)\right] \frac{1}{E}$$

$$= \frac{e^{PS}}{EE} * \ell n\left(\frac{E2}{E1}\right)\left[1 + \frac{XY + 1}{2}\ \ell n(E1 * E2)\right] \quad . \quad (75)$$

From each small energy interval $E1 \leq E \leq E2$ in the integral over the gth group, there will be a contribution to the g´th group, where $g' = 1,\ldots,g$. Therefore, even though it is not explicitly indicated in the notation, quantity B(E) defined in Eq. (62c) and the constants B_0 and B_1 in Eqs. (63) and (64) are dependent on the outgoing group g´. In PROGRAM EVXS, B_0 and B_1 are arrays B0 and B1 into which are stored g values of $B(E_a)$ and $B(E_b)$ for each of the g´ groups. As the range of the incident neutron energy E increases to the point that $E1 = E_b$, the values in the B0 array are replaced by those in the B1 array, and new values for the B1 array are calculated at some new, higher energy E_b. If E should exceed E_{NED}, the highest energy for which an angular distribution is given, we continue with the same values of B_0 and B_1, letting the interpolation become an extrapolation.

The angular distribution integral in Eq. (61) over the range $\Delta\mu(E,g')$ is obtained by taking the difference between the two integrals from -1 to μ_{max} and μ_{min}; viz.,

$$N(E) = \int_{-1}^{\mu_{max}(E,g')} d\mu T(\mu,E)\ P_n(\mu_L)$$

$$- \int_{-1}^{\mu_{min}(E,g')} d\mu T(\mu,E)\ P_n(\mu_L) \quad . \quad (76)$$

The integrals are not evaluated for these limits explicitly, however. Instead, we calculate a set of integrals

$$f_i(E) = \int_{-1}^{\mu_i} d\mu T(\mu,E)\ P_n(\mu_L) \quad (77)$$

where $i = 0,\ldots,NINC$
and

$$\mu_i = -1 + \frac{2i}{NINC} \quad . \quad (78)$$

The integer NINC is the number of intervals into which the scattering cosine range -1 to +1 is divided, and it is read from the angular distribution record. For $\mu_i \leq \mu \leq \mu_{i+1}$

$$\int_{-1}^{\mu} d\mu T(\mu,E)\ P_n(\mu_L) = f_i(E) + (\mu - \mu_i)$$

$$\times \left[\frac{f_{i+1}(E) - f_i(E)}{\mu_{i+1} - \mu_i}\right] \quad . \quad (79)$$

This interpolation is carried out in SUBROUTINE FF. There are NINP = NINC + 1 values for both $f_i(E_a)$ and $f_i(E_b)$ stored in arrays DUTL and DUTP, respectively. The integral over the scattering cosine in Eq. (77) is carried out in SUBROUTINE INTG using Simpson's rule for numerical integration. Simpson's rule is written

$$\int_a^b F(x)\ dx \approx \frac{b - a}{3 \cdot 2 \cdot m} \left[F(x_0) + 4F(x_1) + 2F(x_2) + 4F(x_3) + \ldots + 4F(x_{2m-1}) + F(x_{2m})\right] \quad , \quad (80)$$

where the interval in x from a to b has been divided into 2m intervals, m being an appropriate integer. In our case $F(\mu) = T(\mu,E)P_n(\mu_L)$. We write

$$DUTP_i = f_i(E) = \int_{\mu_0=-1}^{\mu_i} F(\mu)\, d\mu = \left(\frac{\mu_i - \mu_0}{3 \cdot 2 \cdot i}\right)$$

$$\times \left[F(\mu_0) + 4F\left(\frac{\mu_0 + \mu_1}{2}\right) + 2F(\mu_1) + \ldots + 2F(\mu_{i-1}) + 4F\left(\frac{\mu_{i-1} + \mu_i}{2}\right) + F(\mu_i)\right] \quad . \tag{81}$$

The coefficient in round braces can be expressed

$$\frac{\mu_i - \mu_0}{6i} = \frac{-1 + \frac{2i}{NINC} - (-1)}{6i} = \frac{VINC}{3} \quad ,$$

where VINC = 1/NINC. The calculation is arranged in the following way:

$$DUTP_0 = 0.0$$

$$DUTP_1 = \frac{VINC}{3}\left[F(\mu_0) + 4F\left(\frac{\mu_0 + \mu_1}{2}\right) + F(\mu_1)\right]$$

$$\vdots$$

$$DUTP_i = DUTP_{i-1} + \frac{VINC}{3}$$

$$\times \left[F(\mu_{i-1}) + 4F\left(\frac{\mu_{i-1} + \mu_i}{2}\right) + F(\mu_i)\right] \quad . \tag{82}$$

The integrands, as well as the limits of integration in Eq. (76), are determined differently depending on whether the reaction represents elastic or discrete inelastic scattering. However, it is assumed that the angular distribution data for these reactions are always given in the center-of-mass system (SYS = 1). The program proceeds as if this were the case, and only a warning message is printed if SYS = 2. We consider the elastic and discrete inelastic cases separately.

1. Elastic Scattering. The first reaction processed for any material is always the elastic scattering cross section. Thus, for r = 1, ID will always be 2, and we can write explicitly the expression for the elastic group-to-group cross section as

$$\sigma_{l,n,g,g'} = \int_g dE\, \phi(E)\, \sigma_r(E) \times \int_{\Delta\mu(E,g')} d\mu\, T(\mu,E)\, P_n(\mu_L) \quad , \tag{83}$$

where $g' = 1,\ldots, g$ and $n = 0,\ldots, NMAX$.

The integral is carried out over the center-of-mass scattering cosine μ. The argument of the Legendre polynomial in Eq. (83)--cosine of the laboratory scattering angle μ_L--is related to μ through the expression

$$\mu_L = (1 + R3 \cdot \mu)/\sqrt{R1 + R2 \cdot \mu} \quad , \tag{84}$$

where R3 = AM, R2 = 2*AM, R1 = 1 + AM^2, AM = A/1.00866545, and A is the atomic weight of the material. The denominator of the above expression is tested to avoid division by zero. If the quantity inside the radical is less than 0.0001, μ_L is set to zero.

The range of μ allowed for scattering into group g' is

$$\Delta\mu(E,g') = \mu_{max}(E,g') - \mu_{min}(E,g') \quad ,$$

where

$$\mu_{max}(E,g') = \min\left\{+1, \frac{1}{E}\left[E^+_{g'} + \frac{R1}{R2}\left(E^+_{g'} - E\right)\right]\right\}$$

and

$$\mu_{min}(E,g') = \max\left\{-1, \frac{1}{E}\left[E^+_{g'-1} + \frac{R1}{R2}\left(E^+_{g'-1} - E\right)\right]\right\}. \tag{85}$$

These formulas for the minimum and maximum of the cosine of the scattering angle can be derived from simple kinematics for elastic two-body collisions as shown in Jackson[2] and Glasstone,[3] for example. It is plain that the lower boundary for the higher energy group equals the upper boundary for the lower energy group; that is, $\mu_{min}(E,g' + 1) = \mu_{max}(E,g')$. Furthermore, $\mu_{min}(E,g') = -1$ for $g' = 1$. The computation of the limits is done in SUBROUTINE GETMU.

The values of $T(\mu,E)$ required as part of the integrand in Eqs. (77) through (82) are determined in FUNCTION TE. For all energies E such that the probability distributions are tabulated (pairs of μ_i and $T(\mu_i,E)$), linear interpolation in μ is used to determine $T(\mu,E)$. Specifically, for $\mu_i \leq \mu \leq \mu_{i+1}$

$$T(\mu,E) \equiv TE = T(\mu_i,E) + (\mu - \mu_i) \times \left[\frac{T(\mu_{i+1},E) - T(\mu_i E)}{\mu_{i+1} - \mu_i}\right] \quad . \tag{86}$$

The values of μ_i and $T(\mu_i,E)$ are stored in the TK array as described in Sec. II. This function routine can also handle angular distributions expressed in terms of Legendre expansion coefficients. In this case the TK array contains NF coefficients F_n at energy E such that

$$T(\mu,E) = \frac{1}{2}\left[1 + \sum_{n=1}^{NF} (2n + 1)\, F_n\, P_n(\mu)\right] \quad . \tag{87}$$

The Legendre polynomials in Eqs. (77) through (82) with argument μ_L are calculated in FUNCTION PN. It is important to realize that the value of μ passed to the function through the calling sequence is the same μ over which the numerical integration is being carried out. Since μ and $T(\mu,E)$ are in the center-of-mass system, μ_L must be calculated using Eq. (84). If $n = 0$, then $P_0 = 1.0$, regardless of the value of μ. Higher order polynomials are calculated using the recurrence relation*

$$P_n(\mu) = \frac{(2n - 1)\,\mu\, P_{n-1}(\mu) - (n - 1)\, P_{n-2}(\mu)}{n} \quad . \tag{88}$$

For $n < 2$, $P_0(\mu) = 1.0$, and $P_1(\mu) = \mu$.

2. Discrete Inelastic Scattering. In discrete inelastic scattering reactions, the incident neutron loses a certain amount of energy in the scattering, and the energy lost appears in the target nucleus which is left in an excited state. The reaction energy Q_r is negative, and the cross section for each reaction has a definite threshold energy. There is a well defined relationship between the scattering angle and the energy of the secondary neutron. These reactions have $5 \leq ID \leq 14$ and $51 \leq ID \leq 80$ and TYPE = 1; provision has thereby been made for discrete inelastic scattering to as many as 40 excited states of the residual nucleus.

The expression for the nth Legendre component of the scattering matrix for the rth reaction appears to be the same as that for elastic scattering:

$$\sigma_{r,n,g,g'} = \int_g dE\, \phi(E)\, \sigma_r(E) \times \int_{\Delta\mu(E,g')} d\mu T(\mu,E)\, P_n(\mu_L) \quad , \tag{89}$$

where $g = 1,\ldots, G$ and $n = 0,\ldots, NMAX$. The evaluation of this integral proceeds in the same manner as for elastic scattering, but there are some significant differences.

The expressions for $\mu_{max}(E,g')$ and $\mu_{min}(E,g')$ are generalized as follows:

$$\mu_{max}(E,g') = \min\left[+1, \frac{1}{E^*}\left[E^+_{g'} + f \cdot (E^+_{g'} - E)\right]\right]$$

$$\mu_{min}(E,g') = \max\left[-1, \frac{1}{E^*}\left[E^+_{g'-1} + f \cdot (E^+_{g'-1} - E)\right]\right] . \tag{90}$$

The expressions for f and E* are

$$f = \frac{1 + AM^2 - \dfrac{AM(AM + 1)|Q_r|}{E}}{2AM + \dfrac{AM(AM + 1)|Q_r|}{E}} \tag{91}$$

*Substitution of $\ell = n - 1$ in Eq. (3-39) on page 106 of Ref. 4 will give Eq. (88) of this report.

and

$$E^* = \frac{E \cdot \sqrt{AM^2 - \frac{AM(AM+1)|Q_r|}{E}}}{AM + \frac{AM(AM+1)|Q_r|}{2E}} \quad , \qquad (92)$$

where AM = A/1.00866544 as previously and Q_r is the reaction energy. In the limit $Q_r \to 0$, which is the case for elastic scattering, we see that

$$f \to \frac{1 + AM^2}{2AM} = \frac{R1}{R2} \quad \text{and} \quad E^* \to E \quad ;$$

in this limit the expressions in Eq. (90) reduce to those in Eq. (85).

The laboratory scattering cosine μ_L is related to the center-of-mass cosine μ still using the formula

$$\mu_L = \frac{1 + \mu \cdot R3}{\sqrt{R1 + \mu \cdot R2}}$$

in FUNCTION PN, but for discrete inelastic scattering we have

$$R3 = AM \cdot \sqrt{1 - \frac{(AM+1)|Q_r|}{E \cdot AM}} \quad . \qquad (93)$$

At the present time we assume that $T(\mu,E) = 0.5$ in the center-of-mass system for all discrete inelastic reactions. The expression for N(E) becomes

$$N(E) = \frac{1}{2} \int_{\Delta\mu} d\mu \, P_n(\mu_L) \qquad (94a)$$

$$= \frac{1}{2} \int_{\Delta\mu} d\mu_L \frac{d\mu}{d\mu_L} P_n(\mu_L) \quad . \qquad (94b)$$

In practice, we proceed to evaluate the integral as shown in Eq. (94a) using Simpson's integration as discussed in connection with elastic scattering.

In Eqs. (63) and (64) we defined two quantities B_0 and B_1 at energies E_a and E_b for which angular distributions were given. For discrete inelastic reactions we do not use angular distribution data from the library, but assume isotropic scattering in the center-of-mass system at all energies. To make our integration procedure work, we still need NED energies at which to evaluate Eq. (94a). This special set of energies is calculated in SUBROUTINE FINDE.

If n = 0, the integrand in Eq. (94a) is unity, and the integral is evaluated at only two energies

$$E_1 = \frac{AM + 1}{AM} |Q_r| \quad ,$$

the threshold energy, and

$$E_2 = 50 \, E_1 \quad .$$

For n > 0, a special algorithm is used to yield a set of energies E_k with sufficient density to allow the same general integration scheme to be used as for elastic scattering. It is required that the total number of energies NED be between 4 and 20. These energies are calculated in SUBROUTINE FINDE as follows:

$$\begin{aligned}
E_1 &= \frac{AM + 1}{AM} |Q_r| \\
E_2 &= E_1 \cdot \min \left[1 + \frac{0.05}{n+1} , \frac{AM^2}{AM^2 - 1} \right] \\
E_3 &= \left(1 + \frac{0.05}{n+1}\right) E_2 \quad . \\
E_4 &= \left(1 + \frac{0.05}{n+1}\right) E_3 \\
E_5 &= E_4^2 / E_1 \\
&\vdots \\
E_{NED} &= E_{NED-1}^2 / E_1
\end{aligned} \qquad (95)$$

such that $E_{NED-1} < 15 \text{ MeV} \leq E_{NED}$ and $4 \leq NED \leq 20$.

In computing the integral over the gth group in Eq. (89), recall that the energy range E_g^- to E_g^+ is divided into smaller intervals determined by the energies at which the fluxes, cross sections, and angular distributions are tabulated. The boundaries of each small energy interval are E1 and E2, as in Eq. (62). In the discrete inelastic integrations, it is required that E2 shall be large enough that

$$AM^2 > \frac{AM(AM+1)|Q_r|}{E2} \quad ; \qquad (96)$$

otherwise, the integral from E1 to E2 is set to zero. This is really just another way of insuring that the range of integration is above the threshold energy for the reaction and that any integral below the threshold is eliminated.

D. Scattering Computed by Laws

Nonelastic reactions are those for which there is no direct relationship between the scattering angle and the energy of the secondary neutron. The energy distribution of secondary neutrons is described instead in terms of the fractional probability that a neutron of incident energy E will produce neutrons of energy E´. The nonelastic reactions in the LAMDF have identification numbers $15 \leq ID \leq 31$, of which the fission reactions with $18 \leq ID \leq 21$ are a subset. For fission reactions not only the total cross section is calculated for each group, but in addition the fission fractions and the average number of neutrons per fission are calculated. For all other nonelastic reactions, a scattering matrix is calculated.

1. Nonelastic Scattering Matrices. For a nonelastic reaction r with TYPE > 0 and $15 \leq ID \leq 17$ or $22 \leq ID \leq 31$, the expression for the nth Legendre component of the scattering matrix is written

$$\sigma_{r,n,g,g'} = \int_g dE\, \phi(E)\, \sigma_r(E) \times \left[N_{r,g'}(E) \int_{-1}^{+1} d\mu_L T_r(\mu_L,E) P_n(\mu_L) \right] , \quad (97)$$

where $g = 1,\ldots, G$, $g' = 1,\ldots, g$, and $n = 0,\ldots,$ NMAX, the same notation as used in Eq. (58) for elastic and discrete inelastic scattering. The quantity $N_{r,g'}(E)$ represents the fractional number of neutrons scattered into group g´ from the rth reaction induced by an incoming neutron of energy E. It is an integral over the g´th group of the secondary energy probability distribution $p_r(E \to E')$, the fractional probability that for this reaction neutrons of energy E´ will be produced by an incident neutron of energy E. As discussed in Sec. II.D.2 the function $p_r(E \to E')$ may be a tabulated function or it may be a definite analytic function for which parameters are given.

The angular distributions $T_r(\mu_L,E)$ are always given in the laboratory system (SYS = 2) for these reactions. The angular integral in Eq. (97) is over the full range of μ_L from -1 to +1; in comparison with Eq. (58) there is no $\Delta\mu(E,g')$ because we are ignoring energy-angle correlations. If the angular distribution is given in terms of Legendre expansion coefficients, the angular integral becomes especially simple due to the orthogonality of the Legendre polynomials as discussed in Sec. II.D.3. When the angular distribution $T_r(\mu_L,E)$ is tabulated as a function of the scattering cosine μ_L, we first calculate the $F_n(E)$ before proceeding to the integration in energy over group g. Specifically, for each of the NED energies at which $T_r(\mu_L,E)$ is tabulated, we expand the angular distribution as

$$T_r(\mu_L,E) = \frac{1}{2}\left[1 + \sum_{n=1}^{NMAX} (2n+1)\, F_n(E)\, P_n(\mu_L)\right] . \quad (98)$$

Then

$$F_n(E) = \int_{-1}^{+1} d\mu_L\, T_r(\mu_L,E)\, P_n(\mu_L) , \quad (99)$$

precisely the integral over scattering cosine we find in Eq. (97). The procedure used in SUBROUTINE TININ for evaluating the above integral is interesting. Because we work with one reaction at a time and because we evaluate the integral separately for each reaction r and energy E, we can drop the explicit reference to E and r in the following discussion. We also drop the subscript L on μ_L for convenience. It is assumed that linear interpolation is adequate to describe the angular distribution $T_r(\mu)$ between the angles at which it is tabulated. Thus

$$T(\mu) = \frac{\mu_j\, T(\mu_{j-1}) - \mu_{j-1}\, T(\mu_j)}{\mu_j - \mu_{j-1}} + \frac{T(\mu_j) - T(\mu_{j-1})}{\mu_j - \mu_{j-1}}\,\mu \quad (100a)$$

$$= \alpha + \beta\mu \qquad (\mu_{j-1} \leq \mu \leq \mu_j) . \quad (100b)$$

One small part of the integral in Eq. (99) is approximated

$$\int_{\mu_{j-1}}^{\mu_j} d\mu\ T(\mu)\ P_n(\mu) = \int_{\mu_{j-1}}^{\mu_j} d\mu(\alpha + \beta\mu)\ P_n(\mu) \qquad (101a)$$

$$= \alpha \int_{\mu_{j-1}}^{\mu_j} d\mu\ P_n(\mu) + \beta \int_{\mu_{j-1}}^{\mu_j} d\mu\ \mu\ P_n(\mu) \quad . \qquad (101b)$$

The first integral in Eq. (101b) is rewritten using integration by parts:

$$\int d\mu\ P_n(\mu) = \mu\ P_n(\mu) - \int d\mu\ \mu\ P_n'\ \mu \quad .$$

But

$$\mu P_n'(\mu) = P_{n-1}'(\mu) + n\ P_n(\mu) \quad ;$$

therefore,

$$\int d\mu\ P_n(\mu) = \mu\ P_n(\mu) - \int d\mu\ P_{n-1}'(\mu) - \int d\mu\ n\ P_n(\mu),$$

so that

$$\int d\mu\ P_n(\mu) = \frac{1}{n+1}\left[\mu P_n(\mu) - P_{n-1}(\mu)\right] \quad . \qquad (102)$$

The second integral in Eq. (101b) is rewritten using another recurrence relation, again taken from Ref. 4,

$$\mu P_n(\mu) = \frac{1}{2n+1}\left[(n+1)\ P_{n+1}(\mu) + n\ P_{n-1}(\mu)\right] \quad .$$

Thus,

$$\int d\mu\ \mu P_n(\mu) = \frac{n+1}{2n+1} \int d\mu\ P_{n+1}(\mu) + \frac{n}{2n+1} \cdot$$

$$\times \int d\mu\ P_{n-1}(\mu) \quad . \qquad (103)$$

For each angular interval $\mu_{j-1} \leq \mu \leq \mu_j$ in Eq. (101b), we calculate the Legendre polynomials $P_{n+1}(\mu)$, $P_n(\mu)$, and $P_{n-1}(\mu)$ for $\mu = \mu_j$ and μ_{j-1}. Then each Legendre polynomial $P_m(\mu_j)$ is replaced by

$$\int_{\mu_{j-1}}^{\mu_j} d\mu\ P_m(\mu) \qquad (j > 1 \text{ and } m = n+1,\ n,\ n-1)$$

calculated using Eq. (102); Eq. (101b) can then be evaluated as

$$\int_{\mu_{j-1}}^{\mu_j} d\mu\ T(\mu)\ P_n(\mu) = \alpha \int_{\mu_{j-1}}^{\mu_j} d\mu\ P_n(\mu) + \frac{n+1}{2n+1}$$

$$\times \beta \int_{\mu_{j-1}}^{\mu_j} d\mu\ P_{n+1}(\mu) + \frac{n}{2n+1}\beta \int_{\mu_{j-1}}^{\mu_j}$$

$$\times d\mu\ P_{n-1}(\mu) \quad . \qquad (104)$$

These contributions to the total integral over μ from -1 to +1 are calculated and summed to give the Legendre expansion coefficient $F_n(E)$ in Eq. (99). If no angular distribution is specified, i.e., if $TIDR_r < 0$, then the angular distribution is assumed isotropic in the laboratory system and the Legendre expansion coefficient $F_n(E)$ is

$$F_n = \int_{-1}^{+1} d\mu_L\ \frac{1}{2}\ P_0(\mu_L)\ P_n(\mu_L) = \frac{2}{2n+1}\ \frac{1}{2}$$

$$\times \delta_{n,0} \quad . \qquad (105)$$

In Eq. (99) we replaced $T_r(\mu_L,E)$ by 1/2; the factor $P_0(\mu_L) = 1.0$ has been inserted to emphasize the use of the orthogonality relationship for Legendre polynomials. From Eq. (105) we have $F_0 = 1.0$ and $F_n = 0.0$ for $n > 0$, which is as we expect for an isotropic distribution. Of course, for all angular distributions, isotropic or not, $F_0(E) = 1.0$.

Equation (97) can be rewritten as

$$\sigma_{r,n,g,g'} = \int_g dE\ \phi(E)\ \sigma_r(E)\ N_{r,g'}(E)\ F_n(E) \qquad (106)$$

to emphasize that we use the Legendre expansion coefficients in the integral over energy E. As with the absorption integrals, the integration over energy

E is performed numerically be summing the integrals over I smaller intervals in group g. The lower and upper bounds of the I smaller intervals are determined by the energies E_j and E_k at which the cross sections and fluxes, respectively, are tabulated. In addition the intervals are subdivided at whatever incident neutron energies E_m the secondary angular distribution data are given. Let El_i and $E2_i$ be the lower and upper energy boundaries of one of the I intervals. The restrictions just discussed on the boundary limits El_i and $E2_i$ can be summarized by the promiscuous expression

$$E_m \leq E_k \leq E_j \leq El_i \leq E \leq E2_i \leq E_{j+1} \leq E_{k+1} \leq E_{m+1} \quad . \tag{107}$$

Equation (106) is approximated as

$$\sigma_{r,n,g,g'} \approx \sum_{i=1}^{I} N^i_{r,g'}(E_m)\, F_n(E2_i) \int_{El_i}^{E2_i} dE\, \phi(E)\, \sigma_r(E) \quad . \tag{108}$$

The Legendre expansion coefficient F_n is obtained at energy $E2_i$ by linear interpolation between the NED energies at which the coefficients are available. If $E2_i$ is less than E(1), the first energy at which the angular distribution data are given, then $F_n(E2_i) = 0.0$. On the other hand, if $E2_i > E(NED)$, then $F_n(E2_i) = F_n(E(NED))$. The assumption that $F_n(E)$ is approximately constant over the energy interval El_i to $E2_i$ is made because the $F_n(E)$ are slowly varying functions, interpolated between energies much more widely spaced than the separation between El and E2. This situation is insured by requiring that $E2_i < 100El_i$; on the surface this might appear to be no restriction at all, but recall that the energies E(1) and E(NED) are separated by several decades. The simple linear interpolation is carried out in FUNCTION TINEL.

In Eq. (108) an additional superscript i has been added to the quantity $N^i_{r,g'}(E_m)$. This is significant because it is an indication of the special way in which the secondary energy distribution data in the ESJ block are handled. The data and/or parameters for the various laws are given for several incident neutron energies E_m; these are read in SUBROUTINE FTBLN which sets them up for use in the energy range $E_m \leq E \leq E_{m+1}$ as indicated in Eq. (107). There are no contributions to the integral for energies less than $E_{m=1}$, the energy of the first sublist. At all energies above the highest energy E_M in the ESJ block, the sublist corresponding to E_M is used. Thus, for all intervals such that

$$E_m \leq El_i \leq E2_{i'} \leq E_{m+1} \quad , \tag{109}$$

the same sublist in the ESJ block is applicable. Note that i' may be greater than i. For each of the several intervals i to i' in the energy range of this sublist, $N^i_{r,g'}(E_m)$ is reevaluated using $E = (El_i + E2_i)/2$, the average energy over the interval. For certain laws, Law 1 for example, $N^i_{r,g'}(E_m) = N^{i'}_{r,g'}(E_m)$ because the probability energy distribution is independent of the incident neutron energy E. On the other hand, for Law 5, $N^i_{r,g'}(E_m) \neq N^{i'}_{r,g'}(E_m)$ because $g(E,E'/E^q)$ will vary depending on the value of E. New values of $N^i_{r,g'}(E_m)$ are calculated in SUBROUTINE NUMBR for each integration interval in Eq. (108).

As we did in Eq. (48) and those following, let the flux $\phi(E)$ and the rth reaction cross section $\sigma_r(E)$ be expressed

$$\phi(E) = e^P E^X \quad \text{and} \quad \sigma_r(E) = e^S E^Y \quad .$$

Then Eq. (108) is written

$$\sigma_{r,n,g,g'} \approx \sum_{i=1}^{I} N^i_{r,g'}(E_m)\, F_n(E2_i) \times \left[e^{P_i+S_i} \int_{El_i}^{E2_i} dE\, E^{X_i+Y_i} \right] \quad . \tag{110}$$

The term in the square brace in Eq. (110) is written

$$e^{P_i+S_i} \int_{El_i}^{E2_i} dE\ E^{X_i+Y_i} = (E2_i - El_i)$$

$$\times \left[\frac{e^{P_i+S_i}}{E2_i - El_i} \int_{El_i}^{E2_i} dE\ E^{X_i+Y_i} \right] \quad ,$$

where the term in curly braces is the expression for ASUM in Eq. (68) except that E_b and E_a have been replaced by $E2_i$ and El_i. The term in the square brace is evaluated in this way for every interval.

2. Fission Reactions. Fission reactions are a special subset of the nonelastic reactions; they have identification numbers $18 \leq ID \leq 21$, although at this time only reactions with ID = 18 and 19 are handled by PROGRAM EVXS as mentioned in Sec. II.D.2 under Law 7. These fission reactions have TYPE = 0 as a matter of convention. The total fission cross section is calculated

$$\sigma_{r,n,g} = \int_g dE\ \phi(E)\ \sigma_r(E) \int_{-1}^{+1} d\mu_L\ T_r(\mu_L,E)\ P_n(\mu_L) \quad ,$$

and because it is assumed that $T_r(\mu_L,E) = 0.5$,

$$\sigma_{r,n,g} = \int_g dE\ \phi(E)\ \sigma_r(E) \qquad (111)$$

for n = 0 only; $\sigma_{r,n,g} = 0.0$ for all $n > 0$. The fission spectrum χ_g is calculated from the secondary energy distribution data specified by the laws, usually Law 3 or Law 7;

$$\chi_g = \int_g dE'\ p(E \rightarrow E') \quad , \qquad (112)$$

where χ_g represents the fraction of fission neutrons having energy in the gth group. This vector is independent of the incident neutron energy E. Provision has been made in the code for fission fractions $\chi_{g,g'}$ dependent on the incoming energy spectrum as well. Instead of a vector with G elements we have a G × G matrix (stored in block SS) which can be printed on input option. In addition to the secondary energy distribution data which are used to calculate the χ_g's, the ESJ block contains a series of energy, ν pairs used in calculating the integral

$$(\nu\sigma_r)_g = \int_g dE\ \phi(E)\ \sigma_r(E)\ \nu(E) \quad . \qquad (113)$$

From Eqs. (111) and (113) one can calculate

$$(\bar{\nu})_g = \frac{(\nu\sigma_r)_g}{(\sigma_r)_g} \quad ,$$

the average number of neutrons per fission in the gth group. Equations (111) and (113) are evaluated following the same procedure described for other reactions. The energy interval E_g^- to E_g^+ is broken into many small intervals determined by the energies at which the cross sections, fluxes, and ν are tabulated. These integrals can be evaluated without approximation, because all of the quantities are tabulated as linear segments on log-log plots.

3. Additional Comments About the Laws. For all nonelastic reactions there must be entries in the ESJ array from which are calculated the energy distributions of secondary neutrons. For fission reactions the cross section record contains not only the ESJ values but also pairs of values of E and $\nu(E)$ from which group-averaged values of the average number of neutrons per fission are obtained. It remains to discuss in detail how the $N_{r,g'}(E_m)$ and the χ_g mentioned in the previous section are calculated.

For each of the i energy intervals into which the gth energy group has been subdivided, g values of the factor $N^i_{r,g'}(E_m)$ are required to give the fraction of the total number of neutrons scattered into groups $g' = 1, \ldots, g$; these g factors are stored in the array BO. The steps taken in SUBROUTINE COEF for evaluating the contributions to $\sigma_{r,n,g,g'}$ from the ith energy interval in Eq. (110) are as follows:

(1) Obtain the value for ASUM from SUBROUTINE SSUM.

(2) Multiply ASUM by $(E2_i - El_i)$ and store the result in SUM.

(3) Multiply SUM by $F_n(E2_i)$ which is interpolated from the values of F_n in FUNCTION TINEL; store the result again in SUM.

(4) Multiply SUM by each of the g factors stored in the BO array and add the results to contributions from the other small intervals which are stored in the XSUM array.

Thus the question concerning the procedure followed in calculating $N^i_{r,g'}(E_m)$ amounts to asking how the g numbers in the BO array are calculated.

The sublist in the ESJ array for energy E_m is read once in SUBROUTINE FTBLN and used for all energy intervals in the range $E_m \leq E \leq E_{m+1}$. Provision has been made in SUBROUTINE FTBLN for the eight laws described in Sec. II.D.2, and in the following discussion we use the same notation introduced in that section. The parameters corresponding to the several allowable laws are read and stored in specific arrays for later access by SUBROUTINE NUMBR which is called for each of the i small intervals in the larger energy range. In SUBROUTINE NUMBR the first thing done is to zero out the BO array and to calculate for the ith small interval the average incident neutron energy $\bar{E}_i = (E1_i + E2_i)/2$. The details of how the parameters are handled for the various laws will now be outlined.

Law 1. For $g' = 1, \ldots, g$ we store into B1 (g') the sum of the product of the weight for Law 1 with the fractions f_ℓ of neutrons with secondary energies E'_ℓ such that $E^-_{g'} < E'_\ell \leq E^+_{g'}$;

$$B1(g') = w_1 \sum_\ell f_\ell \qquad (E^-_{g'} < E'_\ell \leq E^+_{g'}) \quad .$$

It is assumed that E^-_1, the low energy boundary of the lowest energy group, is 0.0. Furthermore, the entry in the B1 array for the lowest energy group is adjusted so that

$$\sum_{g'=1}^{g} B1(g') = w_1 \quad .$$

In any case that $|\sum_\ell f_\ell - 1.0| > 0.005$, an error message is printed. Since for Law 1 there is no explicit dependence on the incident neutron energy E, the entries in array B1 are simply transferred to the BO array in SUBROUTINE NUMBR.

Law 2. The parameters D_ℓ, A_ℓ, and f_ℓ for this law are read in SUBROUTINE FTBLN and stored into the F1 array in the following arrangement:

$$\begin{aligned}
F1(1) &= 2\,D_1 \\
F1(2) &= 0.5\,A_1 \\
F1(3) &= w_2\,f_1 \\
F1(4) &= 2\,D_2 \\
F1(5) &= 0.5\,A_2 \\
F1(6) &= w_2\,f_2 \\
&\vdots \\
F1(3\ell - 2) &= 2\,D_\ell \\
F1(3\ell - 1) &= 0.5\,A_\ell \\
F1(3\ell) &= w_2\,f_\ell \quad .
\end{aligned}$$

The weight for Law 2 is w_2. The difference $w_2(1.0 - \sum_\ell f_\ell)$ is added to F1(3ℓ); if $|\sum_\ell f_\ell - 1.0| > 0.005$, an error message is printed. In SUBROUTINE NUMBR the quantity $BO(g')$ is incremented by the amount $w_2 f_\ell$ for $E^-_{g'} < E'_\ell \leq E^+_{g'}$ and $E'_\ell = A_\ell(\bar{E}_i - D_\ell)$. As with Law 1, it is assumed that $E^-_{g'=1} = 0.0$. If there exists any ℓ such that these conditions cannot be satisfied for $g' \leq g$, then an error message is printed. At the risk of repetition, it should be obvious that these contributions to $BO(g')$ change for each small energy interval i because of the change in the average energy $\bar{E}_i$.

Laws 3 and 4. For these laws the forms of the sub-sublists in the ESJ array are identical because the dependence on energy E in Law 4 is introduced through the use of several sublists. Entries in the B1 array which may already be nonzero because of contributions from Law 1 are incremented by the amount $\Delta B1(g')$ obtained by integrating over the continuous energy distribution. The tabulated function is read in SUBROUTINE FTBLN; the integral

$$\Delta B1(g') = w \int_{E_{g'}^-}^{E_{g'}^+} dE' \, f(E')$$

is performed numerically in SUBROUTINE LAWFR using the simple trapezoidal rule. The weight for Laws 3 or 4 is denoted by w in the above expression. The integration mesh is determined only by the energy group boundaries and the points at which the function $f(E')$ is tabulated. Obviously, there are no contributions to the $\Delta B1(g'_{max})$ at energies above the highest energy for which $f(E')$ is tabulated. The quantity

$$\left| \sum_{g'=1}^{g'_{max}} \Delta B1(g') - w \right|$$

is forced to vanish by adjusting $\Delta B1(g'_{max})$. However, if the quantity inside the absolute value sign is greater than 0.005w, an error message is printed. The index g'_{max} should not be greater than g because E' should never be greater than E in the LAMDF. Because we have calculated additions to the B1 array, these results are automatically transferred to the B0 array when the B1 array is shifted in SUBROUTINE NUMBR.

If Law 3 or 4 is used to describe the energy distribution of fission neutrons, then $g'_{max} = G$ and the $\Delta B1(g')$ are transferred to the S1 array in which the fission fractions χ_g are stored.

Laws 5 and 6. These two laws are identical in form except that q = 1/2 and 1, respectively, for Laws 5 and 6 in the expression $g(E,E'/E^q)$; this function is tabulated as a function of x, where $x = E'/E^q$. In SUBROUTINE FTBLN we store the tabulated function in array F0 as follows:

$$\begin{aligned}
&F0(1) = 0.0 \\
&F0(2) = w \\
&F0(3) = x_1 \\
&F0(4) = 1/2 \; w \; g(E,x_1) \\
&\quad \vdots \\
&F0(K-1) = x_I \\
&F0(K) = 1/2 \; w \; g(E,x_I) \\
&F0(K+1) = -4.0 \quad .
\end{aligned}$$

Here, w is the weight for either Law 5 or 6. If both laws are used, the data for Law 6 follow those for Law 5 in the same format. In SUBROUTINE NUMBR the integral is evaluated numerically in x space between limits $x_{g'}^-$ and $x_{g'}^+$ where $x_{g'}^- = E_{g'}^-/\bar{E}_1^q$ and $x_{g'}^+ = E_{g'}^+/\bar{E}_1^q$. The integration is carried out from x_1(=F0(3)) to x_{max}, which is calculated taking into account the Q value for the reaction; since $E'_{max} = \bar{E}_1 + Q = \bar{E}_1 - |Q|$, then $x_{max} = (\bar{E}_1 + Q)/\bar{E}_1^q$. The integrals over each of the g' groups are stored in the B3 array;

$$B3(g') = w \int_{x_{g'}^-}^{x_{g'}^+} dx \; g(E,x) \quad .$$

The values of $B3(g')$ are then added to the numbers in the B0 array, but only after they have been renormalized so that

$$\sum_{g'=1}^{g} B3(g') = w \quad .$$

Law 7. The parameters α, b, c, and E_f of the generalized fission spectrum as written in Eq. (33) are read in SUBROUTINE FTBLN. Control is immediately transferred to SUBROUTINE NAY where it is required that α = b = 0. The integral

$$S1(g') = \frac{2}{\sqrt{\pi}} \frac{1}{B^{3/2}} \int_{E_{g'}^-}^{E_{g'}^+} dE' \, \sqrt{E'} \, e^{-E'/B}$$

$$(g' = 1,\ldots,G) \qquad (114)$$

is required. As indicated in Eq. (114), the results for G groups are stored directly into the S1 array where the fission fractions χ_g are found. Equation (114) can be rewritten after dropping the primes on E as

$$\chi_g \equiv S1(g) = \frac{2}{\sqrt{\pi}} \frac{1}{B^{3/2}} \int_0^{E_g^+} dE \sqrt{E} \, e^{-\frac{E}{B}} - \frac{2}{\sqrt{\pi}} \frac{1}{B^{3/2}} \times \int_0^{E_g^-} dE \, \sqrt{E} \, e^{-\frac{E}{B}} \quad .$$

But

$$\frac{2}{\sqrt{\pi}}\,\frac{1}{B^{3/2}}\int_0^E dE'\,\sqrt{E'}\;e^{-\frac{E'}{B}} = \operatorname{erf}\sqrt{\frac{E}{B}} - \frac{2}{\sqrt{\pi}}\sqrt{\frac{E}{B}}\;e^{-\frac{E}{B}}$$

so that

$$\chi_g = \operatorname{erf}\sqrt{\frac{E_g^+}{B}} - \operatorname{erf}\sqrt{\frac{E_g^-}{B}} - \frac{2}{\sqrt{\pi}} \times \left[\sqrt{\frac{E_g^+}{B}}\;e^{-\frac{E_g^+}{B}} - \sqrt{\frac{E_g^-}{B}}\;e^{-\frac{E_g^-}{B}}\right] .$$

We force the normalization to unity,

$$\sum_g \chi_g = 1.0 \quad ,$$

by calculating the fission fraction for the Gth group as

$$\chi_G = 1.0 - \sum_{g=1}^{G-1} \chi_g \quad .$$

The lower energy boundary of the first group $E_{g=1}^-$ is assumed to be 0.0. Law 7 is used only for fission reactions, and since SUBROUTINE NUMBR is never called for such reactions, there is no need to provide for that law in the aforementioned subroutine.

Law 10. There is but one parameter read from the sub-sublist for this law, the quantity a in the expression $T = \sqrt{E}/a$ for use in Eq. (40) and Eq. (115). In SUBROUTINE FTBLN the weight w_{10} for Law 10 is stored in F2(1) and a is stored in F2(2). In SUBROUTINE NUMBR contributions are calculated and added directly to the BO array for each of the g′ groups; viz.,

$$\Delta BO(g') \propto \frac{1}{T^2}\int_{E_{g'}^-}^{E_{g'}^+} dE'\,E'\,e^{-\frac{E'}{T}}$$

$$(g' = 1,\ldots,g) \quad . \tag{115}$$

Here, as in Laws 5 and 6, the Q value for the reaction is taken into account when calculating the maximum allowed value of E′. Thus $E'_{max} = \bar{E}_i + Q$. As indicated in Eq. (115) the $\Delta BO(g')$ are proportional to the integral of the evaporation spectrum over the g′th group. However, the normalization condition requires that

$$\sum_{g'=1}^{g} \Delta BO(g') = w_{10} \quad ,$$

which leads to the introduction of a normalization factor. It is easy to show using integration by parts that

$$\frac{1}{T^2}\int_0^E dE'\,E'\,e^{-\frac{E'}{T}} = 1 - \frac{1}{T}(E+T)\,e^{-\frac{E}{T}} \quad ,$$

so that

$$\Delta BO(g') = \frac{w_{10}}{1 - e^{-\frac{a}{\sqrt{\bar{E}_i}}(\bar{E}_i+Q)}\left[1 + \frac{a}{\sqrt{\bar{E}_i}}(\bar{E}_i + Q)\right]} \times \left\{\left(\frac{aE_{g'-1}^+}{\sqrt{\bar{E}_i}} + 1\right) e^{-\frac{aE_{g'-1}^+}{\sqrt{\bar{E}_i}}} - \left(\frac{aE_{g'+1}^+}{\sqrt{\bar{E}_i}} + 1\right) e^{-\frac{aE_{g'}^+}{\sqrt{\bar{E}_i}}}\right\}. \tag{116}$$

In contemplating Eq. (116) it is well to remember that $\bar{E}_i$ is the average incident neutron energy corresponding to one of the i small intervals in the integration over energy E in Eq. (110). It is the analytic properties of the evaporation spectrum in secondary energy E′ that allowed us to arrive at the expression for $\Delta BO(g')$ in closed form as shown here. Again, it is understood that $E_{g'=1}^- = 0.0$.

Finally, we have a provision in the code to care for such cases where there might not be a law specified at all! Parameters for Law 2 are set up in SUBROUTINE FTBLN as follows:

F1(1) = -2*Q
F1(2) = 0.5/TYPE
F1(3) = TYPE .

This is equivalent to saying that the total available secondary neutron energy E + Q is distributed evenly among the TYPE secondary neutrons.

E. Transport Approximations and the Cross-Section Tables

In Parts A through D of Sec. III we have discussed how, for a single material, the Legendre components of the cross sections for the various types of reactions are calculated. The calculations for a single material are not complete, however, until we combine the multigroup reaction cross sections and scattering matrices into various formats suitable for input to neutron transport calculations; for example, the DTF-IV[5] format. Although Ref. (5) refers to the DTF-IV transport code, it should be understood that the cross-section format described therein is widely used and is appropriate for many transport codes. This becomes more obvious when it is realized that cross sections with a variety of special corrections can be put into DTF format. To understand the various ways of combining the reaction cross sections, it may be helpful to discuss generally how the multigroup-averaged cross sections are handled once they have been calculated in SUBROUTINE COEF.

The cross sections calculated for each reaction in SUBROUTINE COEF and stored in the XSUM array are transferred to the SS array in SUBROUTINE PRTGG. One significant change is made--a change which across the years has been the source of untold confusion for those involved with multigroup processing codes--the cross sections are stored so that group 1 corresponds to the highest energy group and group G to the lowest energy group. All the printed and punched output conforms to this convention, whereas all input quantities follow the convention that group 1 is the lowest energy group. The number of entries in the SS array varies depending on the type of reaction.

(a) For absorption reactions, only G values of the total cross section $\sigma_{r,g}$ are calculated, and these G values are stored in SS(K,1), K = 1,...,G. Any cross section less than 1.0×10^{-6} barn is set to zero. After these values are printed on the output file MTAP = 2, they are stored into extended core storage (ECS) for future reference.

(b) For elastic, discrete inelastic, and nonelastic reactions, except fission, a scattering matrix is calculated for each Legendre component P_0 to P_{NMAX-1}. The storage array for each scattering matrix is dimensioned G × (G + 1), the first column being reserved for the total cross section $\sigma_{r,n,g}$; the second column for the self-scatter cross section $\sigma_{r,n,g,g}$, and the remaining G-1 columns for the downscatter terms $\sigma_{r,n,g,g'}$. Specifically,

SS(1,1) = $\sigma_{r,n,G}$, the total cross section for the highest energy group;

SS(1,2) = $\sigma_{r,n,G,G}$, the self-scatter term for the highest energy group;

SS(1,G+1) = $\sigma_{r,n,G,1}$, the cross section for downscattering from the highest to the lowest energy group;

SS(G,1) = $\sigma_{r,n,1}$, the total cross section for the lowest energy group;

SS(G,2) = $\sigma_{r,n,1,1}$, the self-scatter term for the lowest energy group;

SS(G,j) = 0.0 for j = 3,..., G + 1 because these would correspond to upscatter terms which are not calculated in this code.

It is required that every nonzero entry in the matrix be greater than 1.0×10^{-6}. The matrix is scanned by SUBROUTINE SCAN to determine j_{max}, the smallest value of j, such that for any i, SS(i,j) = 0 for $j > j_{max}$. The matrix SS(i,j) is then printed in the output for i = 1 to G and j = 1 to j_{max}. The full SS matrix is transferred to ECS for each Legendre component. In computing transport-corrected cross sections only the total scattering cross section $\sigma_{r,NMAX,g}$ is calculated for the P_{NMAX} Legendre component; this is stored and printed just as though it were an absorption cross section and occupies only G words in the SS array. The total number of ECS storage words required by any reaction for which scattering matrices are calculated is, therefore, G(G + 1)NMAX + G.

(c) For fission reactions three arrays are passed to SUBROUTINE PRTGG from SUBROUTINE COEF: the S1 array contains the fission fractions χ_g calculated in SUBROUTINES LAWFR or NAY, the S2 array contains values of $(\nu\sigma_f)_g$, and the XSUM array contains values of $(\sigma_f)_g$. Any values less than 1.0×10^{-6} in absolute value are set to zero. The

numbers are stored in three columns of the SS array so that

$$SS(1,1) = (\sigma_f)_G \ , \quad SS(1,2) = (\nu\sigma_f)_G \ , \quad SS(1,3) = \chi_G \ ,$$
$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$
$$SS(G,1) = (\sigma_f)_1 \ , \quad SS(G,2) = (\nu\sigma_f)_1 \ , \quad SS(G,3) = \chi_1 \ .$$

Before these three columns of the SS array are stored in ECS, the average value of ν, $\bar{\nu}$, for each group is calculated and σ_f, $\nu\sigma_f$, $\bar{\nu}$, and χ are printed for each group.

Special attention must be given to the sequence of events if the fission fractions χ are to be dependent on the incident neutron energy E. As mentioned in Sec. III.D.2, we would write χ as a G × G matrix representing for any incident neutron group g the fraction of fission neutrons with secondary energy E´ in group g´. In the original MANIAC code the fission fractions χ_g were calculated using the parameters in the ESJ sublist for energy E_m, where $E_m \leq E_G^+$. The dependence of χ_g on incident neutron energy was thereby ignored--often the case in present-generation multigroup processors. This option is still available in EVXS by setting the input parameter KF = 1. Provision has also been made for a two-dimensional χ calculation which is carried out in SUBROUTINE FTBLN after the fission fractions for a particular E_m have been calculated in SUBROUTINES LAWFR or NAY. The fission fractions $\chi_{g,g'} = 0.0$ for all g such that $E_g^+ \leq E_{m=1}$, the first energy for which secondary energy distribution data are given. In the case $E_m \leq E_g^- < E_g^+ \leq E_{m+1}$, $\chi_{g,g'} = \chi(E_m,g')$, where $\chi(E_m,g')$ represents the values of the fission fractions calculated using the sublist for E_m. In cases where $E_g^- < E_m < E_g^+$, the contributions to $\chi_{g,g'}$ are weighted according to the energy interval over which the ESJ sublist is applicable. Specifically,

$$\chi_{g,g'} = \chi(E_{m-1},g') \frac{E_m - E_g^-}{E_g^+ - E_g^-} + \chi(E_m,g') \frac{E_g^+ - E_m}{E_g^+ - E_g^-}$$

$$(E_g^- < E_m < E_g^+) \quad \text{and} \quad (g,g' = 1,\ldots,G) \ . \tag{117}$$

As discussed under Laws 3, 4, and 7 in Sec. III.D,3, the $\chi(E_m,g')$ are normalized so that

$$\sum_{g'=1}^{G} \chi(E_m,g') = 1.0 \ .$$

Therefore,

$$\sum_{g'=1}^{G} \chi_{g,g'} = 1.0 \ ,$$

and

$$\sum_{g=1}^{G} \sum_{g'=1}^{G} \chi_{g,g'} = G \ .$$

In SUBROUTINE FTBLN the $\chi_{g,g'}$ matrix is stored in the SS array. The average value of $\bar{\chi}_{g'}$ is obtained by averaging $\chi_{g,g'}$ over the incoming energy groups represented by the first subscript g; viz.,

$$\bar{\chi}_{g'} = \sum_{g=1}^{G} \chi_{g,g'}/G \ . \tag{118}$$

These values of $\bar{\chi}_{g'}$ are stored in the S1 array. In SUBROUTINE PRTGG if KF = 2, the SS array in which the $\chi_{g,g'}$ matrix is stored is printed immediately. Then, and only then, are the values of $(\sigma_f)_g$, $(\nu\sigma_f)_g$, and $\bar{\chi}_g$ stored into the first three columns of the SS array.

It remains to describe SUBROUTINE FINIS in which the cross sections for all the reactions are read from ECS and combined according to one of three recipes chosen on input option. Then cards are produced in DTF format according to one of several conventions. The procedure for combining the reaction cross sections depends on input parameters IPN and IW4.

(1) If IPN = 1, consistent P_n cross sections are produced.

(2) If IPN = 0 and IW4 = 0, transport-corrected cross sections are produced in accordance with the prescription by Bell, Hansen, and Sandmeier.[6]

(3) If IPN = 0 and IW4 = 1, the cross sections are transport-corrected in accordance with the practice of Group TD-4 at LASL.

The number of Legendre components, or "tables," calculated depends on the input parameters ISO and IK. The degree of anisotropy is indicated by ISO. If IK = 0, only ISO tables are prepared; if IK = 1, there will be 1 + 2 + ... + ISO tables prepared corresponding to all possible degrees of anisotropy from 1 to ISO. The P_n tables for different values of ISO differ only for transport-corrected cross sections (IPN = 0).

The first table, the P_0 table, contains values of σ_{abs}, $\nu\sigma_{fission}$, and $\sigma_{transport}$, as well as the P_0 scattering matrix for $\sigma_{g\to g'}$. All higher order tables contain only the scattering matrix for the particular table. The absorption cross section for group g is defined as

$$\sigma_g^{abs} = \sum_{r=1}^{R} \sigma_{r,g}^{TYPE_r=0} + \sum_{r=1}^{R} (1 - TYPE_r) \times \sigma_{r,o,g}^{TYPE_r>0} \quad . \tag{119}$$

Included in the summation are total cross sections for absorption reactions (TYPE = 0) from Eq. (47), total nonelastic scattering cross sections from Eqs. (97) and (59) for n = 0, and total fission cross sections from Eq. (111). The downscatter terms of the scattering matrix for the P_n table are obtained by summing the appropriate terms for each reaction;

$$\sigma_{g\to g'}^{n} = \sum_{r=1}^{R} \sigma_{r,n,g,g'} \qquad (g' < g) \quad . \tag{120}$$

Equations (119) and (120) hold, regardless of the maximum degree of anisotropy or the transport approximation.

For consistent P_n cross sections

$$\sigma_g^{transport} \equiv \sigma_g^{total} = \sum_{r=1}^{R} \sigma_{r,g}^{TYPE_r=0} + \sum_{r=1}^{R} \times \sigma_{r,o,g}^{TYPE_r>0} \quad , \tag{121a}$$

and

$$\sigma_{g\to g}^{n} = \sum_{r=1}^{R} \sigma_{r,n,g,g} \quad . \tag{121b}$$

Thus, the P_n table for consistent P_n cross sections is the same, regardless of the degree of anisotropy. Note that NMAX $\geq$ ISO.

For transport-corrected cross sections $\sigma_g^{transport}$ and $\sigma_{g\to g}^{n}$ differ depending on the degree of anisotropy K ($\leq$ ISO) and depending, of course, on the method of effecting the transport correction. If IPN = 0 and IW4 = 0, the Bell, Hansen, Sandmeier[6] approximation for transport correction is used; there

$$\sigma_g^{transport} = \sum_{r=1}^{R} \sigma_{r,g}^{TYPE_r=0} + \sum_{r=1}^{R} \sigma_{r,o,g}^{TYPE_r>0} - \sum_{r=1}^{R} TYPE_r \, \sigma_{r,K,g} \tag{122a}$$

and

$$\sigma_{g\to g}^{n} = \sum_{r=1}^{R} \sigma_{r,n,g,g} - \sum_{r=1}^{R} TYPE_r \, \sigma_{r,K,g} \quad . \tag{122b}$$

The P_n table depends on K because of the K dependence in the last summation. For this option NMAX $\geq$ ISO. If IPN = 0 and IW4 = 1, the transport-corrected cross sections are calculated as

$$\sigma_g^{transport} = \sum_{r=1}^{R} \sigma_{r,g}^{TYPE_r=0} + \sum_{r=1}^{R} \sigma_{r,o,g}^{TYPE_r>0} - \sum_{r=1}^{R} TYPE_r \, \sigma_{r,K,g,g} \tag{123a}$$

and

$$\sigma_{g\to g}^{n} = \sum_{r=1}^{R} \sigma_{r,n,g,g} - \sum_{r=1}^{R} TYPE_r \, \sigma_{r,K,g,g} \quad . \tag{123b}$$

Before they are punched, the cross sections calculated under this option are multiplied by the factor N/A, where N is Avogadro's number and A is the atomic mass number. Careful attention must be paid to the last summation in Eqs. (123a and b). The correction is effected using the self-scatter term for the Kth table and NOT the total scattering cross section $\sigma_{r,K,g}$. Now, EVXS is set up to calculate only $\sigma_{r,n,g}$ for n = NMAX; therefore, to calculate using the TD-4 transport correction it is essential that NMAX $\geq$ ISO + 1.

The quantities σ_g^{abs}, $(\nu\sigma_f)_g$, $\sigma_g^{transport}$, and $\sigma_{g\to g}^n$, are calculated one table at a time and stored in arrays SF, ST0, and ST1 which then are printed on the output file. Finally, numerical values in these arrays must be arranged in DTF format in preparation for output in 80-column BCD format. A few details concerning the format are in order. Each "table" corresponding to one Legendre component is a matrix consisting of G columns, ITL in length. The table length ITL is specified in the input; its default value is G + 3. Within any column corresponding to one of the G groups, we specify IHT, the position of the transport or total cross section, and IHS, the position of the self-scatter cross section. All other entries are positioned relative to these, as shown in Table VIII. Usually, one has IHT = 3 and IHS = 4, in which case the upscatter terms, none of which is calculated in EVXS anyway, are eliminated and there are no empty positions at the head of the column. The default value for ITL is G + 3; if ITL = G + 3 and IHS = 4, then j in Table VIII is G - 1, just the length required to include all possible downscatter terms. If ITL and IHS are chosen so that j < G - 1, the downscattering beyond the limits imposed by this table length is handled in one of two ways, depending on input variable ITBL. If ITBL = 0, the cross-section matrix is "floored"; no scattering is permitted below the lowest energy group allowed by the table length and all entries along the diagonal referring to a single initial group are added to the last-allowed initial group. Thus,

$$\sigma_{g-j\to g}^n \text{ is replaced by } \sigma_{g-j\to g}^n + \sum_{i>g} \sigma_{g-j\to i}^n \quad . \qquad (124)$$

TABLE VIII

ONE COLUMN OF A CROSS-SECTION TABLE

Position	Entry		
1			
.	Blanks		
.			
IHT - 2	σ_g^{abs}		
IHT - 1	$(\nu\sigma_f)_g$		
IHT	σ_g^{tr}		
.		}	Upscatter terms
.			
.			
IHS - 1	$\sigma_{g+1\to g}^n$		
IHS	$\sigma_{g\to g}^n$		Self-scatter term
IHS + 1	$\sigma_{g-1\to g}^n$	}	Downscatter terms
IHS + 2	$\sigma_{g-2\to g}^n$		
.			
.			
.			
ITL	$\sigma_{g-j\to g}^n$	j = ITL - IHS	

Equation (124) shows the procedure followed for the MANIAC code. If ITBL = 1, the cross-sections matrix is "truncated" and all scattering below the lowest allowed energy group is treated as absorption so that

$$\sigma_g^{abs} \text{ is replaced by } \sigma_g^{abs} + \sum_{i>g} \sigma_{g-j\to i}^n \quad . \qquad (125)$$

In either case neutron balance is maintained. If the sum of the remaining terms below the cutoff, the summations in Eqs. (124) or (125), amounts to less than 0.001% of the transport cross section for that particular group, the cutoff terms are simply ignored.

The elements of each scattering table are stored in a column vector ITL × G in length, ITL numbers for each group as shown in Table VIII. This vector is then written in BCD format (six floating point numbers per card plus sequencing information) onto the output tape and onto a scratch file TAPE4. This disk file can then be punched using the PUNCHIT

control card available at LASL or by setting up the PUNCH file in the PROGRAM card and adding the equivalence TAPE4 = PUNCH. For a single table there will be (ITL*G/6) + 1 cards punched. Sometimes, the repetition of many zeroes in the tables results in a rather bulky card output. This problem can be circumvented by use of the ANISN[7] format; special control flags are punched preceding the repeated numbers to indicate how many times the numbers would be found successively in a vector array. Other special format options are available through the IW4 input flag. These options make use of SUBROUTINES PUNREP and PUNCL prepared for use at LASL by Forrest Brinkley of Group T-1.

F. Nonfission Neutron and Gamma Energy Deposition

In weapons vulnerability and radiation shielding problems at LASL there is interest in material heating caused by nonfission neutrons and neutron-induced gamma rays. To calculate the energy deposition due to incident neutrons, one must know the individual reaction cross sections and the Q values for each reaction. This information is included in the heating numbers H_g which are defined such that the product $\phi_{i,g} H_g$ gives the amount of energy deposited by the incoming neutron beam; $\phi_{i,g}$ is the neutron flux (neut/cm^2) at space point i for neutron energy group g; H_g is the heating number for neutron energy group g in (cal/kg per neut/cm^2) $\times 10^{-13}$. A complete discussion of the energy deposition problem is available in Refs. (8) and (9), where it is shown that H_g for one reaction is calculated

$$H_g = \frac{230.5}{A} \sigma_{r,g} \bar{E}_g \quad \left(\frac{\text{cal/kg}}{\text{neut/cm}^2} \times 10^{-13} \right) \quad ;$$

$\sigma_{r,g}$ is the total reaction cross section, $\bar{E}_g$ is the median energy for group g, and A is the atomic mass. The EVXS code has been modified to calculate appropriate heating terms. The calculations, which are performed in SUBROUTINE SSS, are carried out if IW4 = 2 and IPN = 1 for any material.

For each reaction the following quantities are computed and printed for each group:

$$f_{r,g} = \sigma^{tot}_{r,g} * \bar{E}_g \quad ,$$

$$f_{r,q} = \sigma^{tot}_{r,g} * Q_r \quad ,$$

$$\hat{f}_{r,g} = \bar{E}_g \sum_{g'=1}^{g} \sigma_{r,o,g,g'} \quad ,$$

$$\hat{f}'_{r,g} = \sum_{g'=1}^{g} \bar{E}_{g'} \sigma_{r,o,g,g'} \quad ,$$

$$f^{tot}_{r,g} = \frac{230.5}{A} \left[f_{r,g} + f_{r,q} - \hat{f}'_{r,g} \right] \quad ,$$

where $\bar{E}_g$ is the median energy for group g and is given in the library as part of the group structure information. The first quantity $f_{r,g}$ is the H_g number for the reaction multiplied by the factor A/230.5; $f_{r,q}$ represents the energy loss due to the inelastic nature of the reaction; $\hat{f}'_{r,g}$ includes the kinetic energy of the secondary neutrons produced in the reaction. Thus, the quantity $f^{tot}_{r,g}$ is related to the kinetic energy of the charged particles and gamma rays produced by the reaction. This would be the total energy deposition if all gamma rays were absorbed in the material. After the quantities $f^{tot}_{r,g}$ have been calculated for all reactions, they are summed to give the total energy deposition for all gammas absorbed, GA_g.

To get an estimate of the amount of energy deposited due to the kinetic energy of the charged particles, we subtract from GA_g a quantity proportional to the group-averaged gamma energy production cross section, GI_g. The array GI is read in to EVXS and multiplied by the factor 230.5/A to give GP_g. Finally, to obtain the total energy deposition when all gammas leak out, GD_g is calculated; viz., $GD_g = GA_g - GP_g$. All of these heating quantities are printed in the summary output.

IV. DESCRIPTION OF THE CODE

A. Overall Operation

A diagram indicating the relationship of the principal subroutines in this program is given in Fig. 3. The subroutines have been arranged on four "levels," depending on the frequency with which they are called; the more frequently called subroutines are placed on a lower level in the figure.

1. EVXS--Overall Control. The overall control of the flow in this code is governed by PROGRAM EVXS. The main program serves to define the length

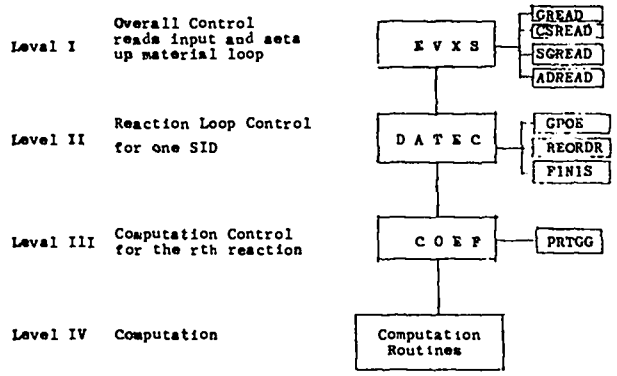

Fig. 3. Arrangement of principal subroutines.

of unlabelled common, of course, and to set up the necessary disk files. The input data are read to determine for which materials multigroup cross sections are to be calculated and which group structures are desired. The first file of the library is then read by SUBROUTINE GREAD to find the desired group structure sets and to store them into ECS for future use. At this point any group structures that are to be taken from cards are also read by GREAD and stored into ECS. Materials for which no group structures are found are eliminated from the problem after a comment has been printed.

The rest of the main program consists of a large loop over the remaining requested materials. The identification, or SID, number of each of the remaining files in the LAMDF is read and compared with the SID numbers requested. If there is a match, the first record of the cross-section file is read by SUBROUTINE CSREAD and the energies at which the cross sections are tabulated are stored into ECS. The cross-section records for the R reactions are read by SUBROUTINE SGREAD and stored into ECS; finally, the ND angular distribution records for material SID are read by SUBROUTINE ADREAD and the energies, probability distribution data, and range indicators are stored into ECS. Control is then transferred to SUBROUTINE DATEC which supervises the group-averaging of the cross sections for all reactions. If there is no match when the identification number SID is read from the first record in the cross-section file, the remainder of the file is skipped and the identification number of the next file is read again, matching against the materials requested. Thus the code proceeds through the LAMDF until multigroup cross sections for all requested materials have been calculated or until the end of the library tape has been reached.

2. DATEC--Reaction Loop Control for One Material. The control of the multigroup averaging of the reaction cross sections for one material lies in SUBROUTINE DATEC. It reads the appropriate group structure from ECS and calls SUBROUTINE GPOE where the X_i and P_i of Eqs. (50) and (51) are calculated and stored in arrays X and POE. Next, a loop over all reactions is executed in which the cross sections, the secondary energy distribution data, and the appropriate set of angular distributions for a single reaction are read from ECS into arrays in unlabelled common. Before the cross sections are stored into the SIG array, they are shifted by SUBROUTINE REORDR so that the values are in positions corresponding to those of the energy array ES. The values for the highest and lowest energies for which the cross sections are defined are extended to the highest and the lowest energies for which the energy mesh is given. These values should normally be zero but, to handle the log-log interpolation, 10^{-20} is used. The calculation of the multigroup-averaged cross sections for each reaction is carried out in SUBROUTINE COEF which is called from DATEC.

After the cross sections for all reactions have been calculated, printed, and stored into ECS, SUBROUTINE FINIS is called; this routine retrieves the group-averaged reaction cross sections from ECS and builds up the Legendre components of the scattering tables in DTF[5] format. Five subroutines are called by FINIS:

(a) SUBROUTINE SCAN checks every scattering table to determine which values of the scattering matrix can be regarded as within the level of significance of the methods used in the code, i.e., greater in absolute value than 10^{-6} barn.

(b) SUBROUTINE PRTB prints scattering tables in the output.

(c) SUBROUTINE CARDS writes the scattering tables in BCD card image format on unit LTAP = 4.

(d) SUBROUTINES PUNREP and PUNCL create special BCD card images appropriate for input to the ANISN[7] and DTF[5] loaders. These routines were written by Forrest Brinkley of LASL.

(e) SUBROUTINE NEWPG restores the page on the output file and prints a page header including the date and the description of the material being processed as found in the array SDES (8).

After all the scattering tables have been prepared, control is returned from FINIS to DATEC, where a check is made to see whether calculations with the same SID are to be made with different parameters. If so, the calculation is carried out; if not, control is returned to EVXS.

3. COEF--Computation Control for One Reaction. The computation of multigroup-averaged cross sections, as discussed in detail in Sec. III, is carried out in SUBROUTINE COEF and 16 other computational routines. In addition to the initial section in which required parameters are set, COEF can be divided into three principal sections whose purposes are to compute absorption reactions, to compute elastic and discrete inelastic reactions, and to compute nonelastic and fission reactions. The particular section to be entered depends on the TYPE and ID for the reaction, as shown in Table V and summarized in Table IX. In the first section we evaluate integrals like those in Eqs. (47) and (48); in the second section we deal with the evaluation of expressions like Eq. (58); the third section is designed to handle expressions such as that found in Eq. (97). There is one thing common to these different expressions: they all involve integration in incident neutron energy between the group boundaries E_g^- and E_g^+; this is the work accomplished in COEF with the aid of SUBROUTINES SPACE and GSOE. The relationship of SPACE and GSOE to COEF is best understood by referring momentarily to Eqs. (48), (49), (52), and (57); the quantity INT in Eq. (57) is evaluated in COEF, but SPACE determines the values of k and j such that $E_k \leq E_i \leq E_{k+1}$ and $E_j \leq E_i \leq E_{j+1}$. The quantities Y_i and S_i defined in Eqs. (53) and (54) are calculated in GSOE once j has been determined in SPACE. The quantities X_i and P_i of Eqs. (50) and (51) were previously calculated and stored by DATEC. SUBROUTINES SPACE and COEF are included among the 16 "computational routines" mentioned in Fig. 3; only these two routines are called from the first principal section of COEF.

TABLE IX

OUTPUT STORAGE REQUIREMENTS FOR VARIOUS CATEGORIES OF REACTIONS

Category	ID	Type	Ang. Dist. Given?	Length ILR_r
Elastic	2	1	Yes	G*GP*NMAX + G
Discrete Inelastic	5 thru 14 51 thru 80	1	No	G*GP*NMAX + G
Fission	18, 19, 20, 21	0, 1, 2	No	3*G
Absorption	101 thru 108	0	No	G
Non-elastic	15 thru 17 22 thru 31	1, 2, 3	Yes No	G*GP*NMAX + G G*GP

Note: G = number of groups from group set GID.
GP = G + 1.
NMAX = maximum order of the Legendre polynomials used.

We have seen in Sec. III that Eq. (58) for elastic and discrete inelastic scattering can be reduced to the sum of a series of integrals over small energy intervals as written in Eqs. (62) and (69). The expression for INT is evaluated in COEF, but the components of the expression are evaluated in the computational routines. Referring to the expressions in Eq. (68), we know that S and Y are evaluated in GSOE; it remains to review how $B_0(\equiv B(E_a))$ and $B_1(\equiv B(E_b))$ in Eqs. (63) and (64) are calculated. The range of μ allowed for scattering into group g' is determined in SUBROUTINE GETMU. The Legendre polynomials $P_n(\mu_L)$ are calculated in FUNCTION PN; the angular distribution function $T(\mu,E)$ is calculated in FUNCTION TE; the NINC integrals for $f_i(E)$ as written in Eq. (77) are calculated in SUBROUTINE INTG. The interpolation of the values of $f_i(E)$ to μ_{min} and μ_{max} is carried out in FUNCTION FF. Having obtained the integrals over the range of μ, B_0 and B_1 are calculated in COEF. Quantities ASUM and BSUM are obtained in SUBROUTINE SSUM and the results are combined in COEF. For discrete inelastic scattering SUBROUTINE FINDE is used to determine energies to use as E_a and E_b according to the formulas in Eq. (95).

The expression in Eq. (97) for nonelastic scattering matrices can be rewritten as shown in Eq. (106) and further approximated as shown in Eq. (110). The expression in square braces in Eq. (110) is evaluated with the aid of SSUM; the Legendre expansion coefficients F_n are obtained at the energies given in the library from SUBROUTINE TININ and interpolated to energies $E2_i$ in FUNCTION TINEL. The secondary energy distribution data are read in SUBROUTINE FTBLN; the fractions $N^i_{r,g'}(E)$ are calculated in SUBROUTINE NUMBR.

For fission reactions the parameters Z and ZOE for use in the expression

$$\nu(E) = e^{ZOE}\, E^{Z}$$

are calculated in SUBROUTINE FISSN. The fission fractions χ_g may be calculated in SUBROUTINES LAWFR or NAY depending on the parameters read by FTBLN.

The results of the calculations in COEF for each reaction are printed by SUBROUTINE PRTGG for each value of n from 0 to NMAX as they are finished; the results then are stored into ECS for retrieval later by FINIS.

4. Other Routines. SUBROUTINE ERROR is called from subroutines at all levels in the code. There are certain non-ASA standard system routines and functions used in the code. These are SUBROUTINES DATE1, CPAREA, ECRD, ECWR, EXIT, ERF, ENCODE, and DECODE.

B. Storage Allocation--ECS and COMMON

Although PROGRAM EVXS is not "variably dimensioned" according to the literal usage of that expression, large blocks of core in ECS and unlabelled common are used for storing those large arrays whose dimensions are not known until the arrays are read. It is not necessary to provide storage for the "worst" possible needs, but instead one can plan on a trade-off in the combination of group structure, cross sections, and output storage demands. The arrays are stored one after another in the large storage block; of course, one must keep track of which location in the large block corresponds to the first word of each array. These location markers are often called "pointers"; they point to the first word of each array. We consider first the arrangement of data in ECS and then turn to the storage of arrays in block AA(21000) in unlabelled common.

The arrangement of data in ECS is shown in Fig. 4. The first block contains the information which is stored into the IA array when the input cards are read by the main program. Since NT, the number of cross-section request cards, may be as large as 20, the IA array requires a block of ECS storage no larger than 200, as indicated under "Comments" in Fig. 4. The group structure information for every GID requested in the input cards is stored next to ECS. If some GID is requested which does not exist on the library tape or in the input

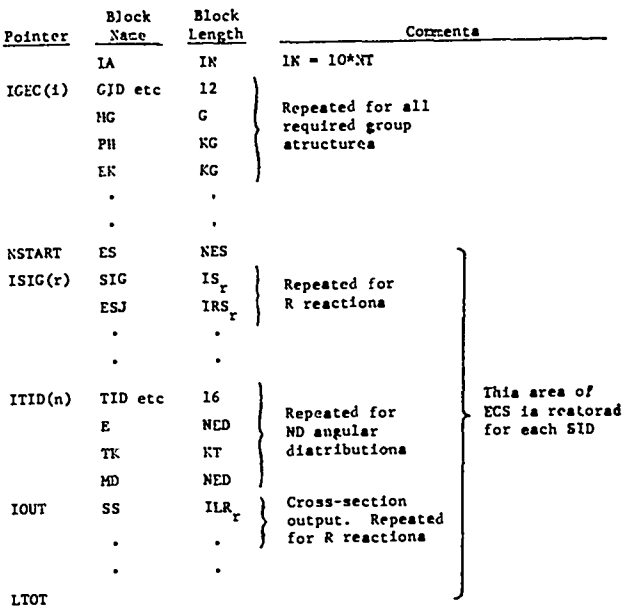

Fig. 4. Arrangement of data in extended core storage.

data, the request is ignored and the program proceeds as though there were NT - 1 materials to be processed. Each GID requires 2*KG + G + 12 words of storage, G being the number of groups and KG the number of flux, energy pairs. The 12 words represented by "GID etc" in Fig. 4 are GID, GDES(8), G, KG, and LGID, where LGID = 2*KG + G. The location of the first word GID in the ith group structure block is saved in IGEC(i). These blocks are stored into ECS in SUBROUTINE GREAD. The order in which the group structure data are stored is not the order in which they are requested but instead the order in which they appear on the library tape.

The pointer NSTART marks the first location of storage used for each SID. The library tape is searched until one of the requested materials is found. In SUBROUTINE CSREAD the first record of the material file is read and the NES energies at which the cross sections are tabulated are stored into ECS, starting at NSTART. In SUBROUTINE SGREAD the cross-section records for the R reactions are read and stored into ECS; the locations of the first words of storage for each record are saved in the ISIG array. Similarly, the angular distribution records are read from the library tape in SUBROUTINE ADREAD and stored into ECS; the pointer words are saved in the ITID array. The 16 words represented

by "TID etc" in Fig. 4 are TID, TDES(8), NED, SY, LEG, KT, NINC, LTID, and A. Finally, ECS locations must be allocated for the output of the calculations. The SS array is the array into which results obtained in SUBROUTINE COEF are stored in SUBROUTINE PRTGG. After the calculations for a given reaction are completed, PRTGG prints the results and stores the contents of SS into ECS. The first word of storage for the first reaction is marked by pointer IOUT. The lengths ILR_r of the output blocks for each reaction r depend on the type of reaction as summarized in Table IX. The last word of ECS storage required is at location LTOT; before the calculations are started, LTOT is calculated to be sure that the ECS requested on the JOB card is sufficient. If it is not, LTOT is printed but the calculations are skipped and we proceed to the next SID.

The large AA(21000) array in unlabelled common is used for core storage of arrays of variable lengths. The arrangement of the arrays, their lengths, and their pointer words are summarized in Fig. 5. With the exception of the SS array, all of these arrays are stored in SUBROUTINE DATEC. The exception, SS, into which data are written in SUBROUTINE PRTGG, is also an exception in that it is the only doubly dimensioned array. If we recall that LGID = 2*KG + G, it can be seen at once that the pointer word IAES = 2*LGID + 1. The first LGID words contain the group structure information read back from ECS into the AA array. Quantities POE and X and P_i and X_i, respectively, of Eqs. (51) and (50); the ESP array contains the values for E_g^+. The ES array contains the energies at which the reaction

Pointer	Array Name	Array Length	Comments		
IMG	MG	G	Read into core from ECS	For a particular GID	
IPH	PH	KG			
IEK	EK	KG			
IPOE	POE	KG	Computed in DATEC		
IX	X	KG			
IESP	ESP	G			
IAES	ES	NES	Cross-section energies		For a particular SID
ISS	SS	G(G + 1)	Output storage		
IEN	E	NED	Angular distribution data	Restored for each reaction	
ITK	TK	KT			
IMD	MD	NED			
ISG	SIG	NES	Values for σ_r		
IESJ	ESJ	IRS_r	Data for laws		

Fig. 5. Arrangement of data in large common storage array AA.

cross sections are tabulated; array SS contains the group-averaged cross sections which are calculated in SUBROUTINE COEF. The next three arrays contain the data for the angular distribution set appropriate for reaction r, and the cross sections and secondary energy distribution data for reaction r are given in the last two arrays. The maximum storage required for any material is calculated in EVXS and DATEC; the total is compared with 21000 to insure the availability of sufficient storage in AA.

C. Definition of Variables

A catalog of most variable names introduced in this program and the subroutines in which they are used is found in this section. Four classes of variables have been considered: integers which serve as temporary indices, counters, or pointers; arrays in which Hollerith data are stored; variables used for temporary storage; and variables used more universally throughout the code.

Integers used locally in various subroutines as temporary indices, counters, and pointers are I, IC, IER, IG, II, IL, IT, J, K, KK, L, LG, L1, L2, N, N1, N2, and N3.

Arrays in which Hollerith data are stored are listed in Table X; the names of the subroutines in which the arrays are used are included in parentheses following the array name.

TABLE X

ARRAYS CONTAINING HOLLERITH DATA

ASTR(EVXS)	IPLUS(PUNCL)
ATMP(FTBLN,LAWFR)	IPOSCF(PUNCL)
FS(ERROR)	IPOSCT(PUNCL)
FTB(FTBLN)	IPSEX(PUNCL)
F1(ERROR)	IPSGN(PUNCL)
F2(ERROR)	ITERCD(PUNREP)
F3(ERROR)	ITERED(PUNREP)
IALLBK(PUNCL)	ITERMC(PUNCL)
IBLNK(PUNCL,CARDS)	LABEL(FINIS)
IHOLAR(PUNREP)	MAIN(EVXS)
IHOLB(PUNREP)	MSR(EVXS)
IHOLDR(PUNREP)	M5(FINIS)
IHOLL(PUNREP,PUNCL)	PRNT(NEWPG,FINIS)
IHOLT(PUNREP	P5(FINIS)
IDC(PUNREP)	SMSG(SSS)
IPIEGN(PUNCL)	WRT(SSS)
IPISNN(PUNCL)	

Certain temporary storage variables have been assigned names for convenience. They are listed in Table XI; the names of the subroutines in which the variables are used are given in parentheses. For variables in this category there is no relationship between quantities with the same name in different subroutines. The word MANY in parentheses refers not to the name of a subroutine but to the fact that the variable appears in many subroutines.

TABLE XI

TEMPORARY STORAGE VARIABLES IN SUBROUTINES

AR(NUMBR)
BT(COEF,FINIS)
ECG(SSS)
EM(FTBLN)
EP(FTBLN)
ESX(LAWFR)
ETMP(COEF)
EX(GPOE,GETMU)
GIN(EVXS,DATEC)
GM(FTBLN)
GP(FTBLN)
ICARDC(PUNCL)
ICILD(PUNCL)
IDEL(SSS)
IDENC(PUNCL)
IDX(PUNREP)
IDXBLD(PUNCL)
IDXILD(PUNCL)
IDXRLD(PUNCL)
IDY(PUNCL)
IGE(EVXS,DATEC,SSS)
IGX(PRTGG,SCAN,FINIS,SSS)
IGN(PRTGG,SCAN,FINIS,PRTB)
IGT(FINIS)
IG4,IG5(FINIS)
IH(FF)
IHSX(EVXS)
IHTX(EVXS)
ILIM(FINIS)
ILL(NUMBR,FINIS)
ILN(FINIS)
IPOSCH(PUNCL)
IPT(ERROR)
IREM(SSS)
IRET(INTG)
IRP(SSS)
ITEMP(PUNREP)
ITERM(PUNCL)
ITLX(EVXS)
IVECR(PUNREP)
IW1(SSS)
IO(FTBLN)
JT(INTG,TE)
LD(ADREAD)
M(TE,PN)
MAX(COEF,FINIS)
MEC(EVXS,DATEC)
MU(PN)
N1,N2,N3,N4(ERROR)
PM,PP(TE,PN)
PZ(TE,PN)
RQT(COEF)
TEMP(EVXS,PRTGG)
TEST(COEF,SSUM,INTG,PRTGG)
TL(INTG)
TMP1(GETMU)
TMP2(GETMU)
TN(NUMBR)
T11(NUMBR)
T1,T2,T3(MANY)
T4(NAY)
T9(NUMBR)
T99(NUMBR)
VINC(INTG)
VK(INTG)
V1,V2,V3,V4,V5,V6(SSS)
XN,XT(NUMBR)
XX(FF)
X1,X2,X3,X4(MANY)
YY(PN)

By far the largest list of names is that for variables which are common to many subroutines. These variables may appear in labelled or unlabelled common statements, or they may be transferred through the calling sequences when control is transferred between subroutines. In Table XII the variables are given, along with their storage locations and definitions. The storage is located most frequently in blank or labelled common; local storage is indicated along with the subroutines in which the variables appear.

TABLE XII

VARIABLES DEFINED UNIQUELY IN PROGRAM EVXS

Name	Storage Location	Definition
A	Blank Common	Mass of target material
AA	Blank Common	Block used to store data from ECS for current material
AF	Local FTBLN,NAY	Input parameter for Law 7 (currently 0)
ALP	Local EVXS	Block to contain input title card
AM	INT Common	=A/1.00866545
AMP	INT Common	=AM * (AM + 1.0) * RQ
AM2	INT Common	$=AM^2$
ASUM	Local COEF,SSUM	First part of the integral for interval from E1 to E2
BB	Local COEF	$=E_j * E_{j-1} * (f(E_{j-1}) - f(E_j))$ or $E2 * BO_g - E1 * B1_g$
BF	Local FTBLN,NAY	Input parameter for Law 7 (currently 0)
BSUM	Local COEF,SSUM	Second part of the integral for interval from E1 to E2
BO	CMPUTE Common	For elastic and discrete inelastic: B(E) for E1
B1	CMPUTE Common	For elastic and discrete inelastic: B(E) for E2
B3	CMPUTE COEF,FTBLN NUMBR	Integral storage block for Laws 5/6
CF	Local FTBLN,NAY	Input parameter for Law 7 (currently 0)
DAT	Blank Common	Date on which processing is done
DF1	Local COEF	=F1X - F1N
DF2	Local COEF	=F2X - F2N
DUTL	CMPUTE Common	Integrals over $d\mu$ for angular distribution energy E_{j-1} (previous)
DUTP	CMPUTE Common	Integrals over $d\mu$ for angular distribution energy E_j (current)
E	Local ADREAD,COEF FINDE,TINEL	Block of angular distribution energies (≤ 400)
EC	Local COEF	Current value of cross-section energy
ED	INT Common	Current value of angular distribution energy
EDL	Local COEF	Previous angular distribution energy
EE	Local COEF,SSUM GETMU,NUMBR	Difference between $E\mu$ of two energies (=E2L - E1L) or between two energies (=ED - EDL)
EF	Local COEF,FISSION	Current energy maximum for fission reaction in computing ν
EG	Local GREAD,COEF	Current energy value for flux function

TABLE XII (Cont.)

Name	Storage Location	Definition
EGM	Local COEF	Lower group energy bound (E_g)
EGP	INT Common	Number of groups plus one (=G + 1)
EK	Local GREAD,GPOE, COEF,SPACE	Block containing energies at which fluxes are given ($\leq$ 500)
EL	INT Common	Upper energy bound for current incoming energy group (E_g^+)
EMAX	Blank Common	Upper energy bound for current law integral
EPS	INT Common	Limit beneath which values are not printed but are considered equivalent to zero (= 10^{-9})
ES	Local CSREAD, COEF, SPACE, GSOE	Block of energy values for which cross sections are given
ESJ	Local SGREAD,COEF, FTBLN, LAWFR, FISSN	Block of data for computation of scattering fractions due to laws
ESP	Local GPOE,COEF, FTBLN,LAWFR, NUMBR,NAY	Block of energies representing upper encrgy bounds for each group (E_{g+})
ESTEP	Blank Common	Formula to determine step size $\left[=1.0 - \left(FAC*\ell n\left(\frac{E1}{EL}\right)\right)/N\right]$
ET	Local FTBLN,NAY	Input parameter for Law 7
ETH	Local COEF	Threshold energy for first non-zero cross section (SIG)
EXL	Local SSUM	=E2L - E1L
E1	INT Common	Lower energy for each energy step in integrating
E1L	Local COEF,SSUM	=ℓn(E1)
E2	Local COEF,NUMBR, TINEL,FISSN	Upper energy for each energy step in integrating
E2L	Local COEF,SSUM	=ℓn(E2)
FAC	INT Common	Preset factor to determine step size for integration (=0.05)
FE	Local GETMU	Temporary storage for function f in computing μ_{min} and μ_{max} in ($E_g^- + f(E_g^- - E)$)
FMT	Local FINIS,CARDS	Block containing format for output of cards and print
FO	Local COEF,FTBLN, NUMBR	Output data block for Laws 5/6
F1	Local COEF,FTBLN, NUMBR	Output data block for Law 2
F2	Local COEF,FTBLN	Output data block for Law 10
FIN,FIX	Local COEF	Linearly interpolated functions of μ_{max} and μ_{min}
F2N,F2X		FIN = $f(\mu_{min}, E_{old})$
G	Blank Common	Number of energy groups
GDES	Blank Common	Description of current group set
GE	Blank Common	Block of weighted group energies
GID	Blank Common	Ident for group set currently being used (=GIDN(NM))
GIDN	Blank Common	Block of group set idents for each material ($\leq$20)
IA	Local EVXS,DATEC	Current position in AA block
IAA	Blank Common	Maximum storage available in AA block (currently 21000)
IAES	Local DATEC	Origin in AA block for ES block for call to COEF
IB	Blank Common	Indicator of type or output requested for PUNREP
IBCDCC	Local PUNCL	Temporary compressed block for storage of characters for words being converted
ICARDX	Local PUNCL	Maximum number of cards
ID	Blank Common	Ident number of reaction currently being processed (= MOD (IDR$_r$,1000))

TABLE XII (Cont.)

Name	Storage Location	Definition
IDIF	Local REORDR	Difference between one and position of first energy for nonzero cross section
IDMAXR	Local PUNREP	Maximum number of repeats
IDN	Local PUNREP	Indicator for next test
IDR	Blank Common	Block of ident numbers of all reactions for current material
IDT	Local PUNREP	Initial test indicator
IE	Local COEF,INTG, PN,GETMU,FF,TE	Trigger for elastic and inelastic: 0 = Elastic 1 = Inelastic, n = 0 2 = Inelastic, n $\neq$ 0
IEC	Blank Common	Current initial position for ECS storage
IEK	Local DATEC	Origin in AA block for EK block for call to COEF
IEN	INT Common	Origin of E block in DATEC; indicator for SPACE in COEF
IEND	Blank Common	Last position in ECS for storing output
IENDR	Local PUNCL	Starting position for current value
IES	Blank Common	Origin in ECS for ES block
IESJ	Local DATEC	Origin in AA block for ESJ block for call to COEF
IESP	Local DATEC	Origin in AA block for ESP block for call to COEF
IFF	Blank Common	Trigger to indicate fission reaction for TYPE = 0, 18 $\leq$ ID $\leq$ 21
IFIN	Local PUNCL	Final position for current value
IFND	Local EVXS	Indicator that requested GID is found
IFO	Local FINIS	Counter of tables done (2 for each pass)
IG	Blank Common	Generally used index for g (group scattered)
IGEC	Blank Common	Block of origins in ECS of group sets for each material (SID)
IGG	Blank Common	=IGP * G
IGP	Blank Common	=G + 1
IGR	Local SSS	Index for weighted group energy
IHS	Local EVXS,FINIS	Position in output table of self-scatter cross section
IHT	Local EVXS, FINIS	Position in output table of total cross section
IIA	Local ADREAD,DATEC	Temporary word for sum of AA block storage needed
IID	Local EVXS,ADREAD	Angular distribution ID numbers for nonelastic reaction
IIG	Local SSS	Index for inner group loop
IK	Local EVXS,TININ, FINIS	Input indicator for number of tables desired: If zero, K-table only (k = ISO); if one, all tables, (k = 1,..., ISO)
IL	Local (Many)	Generally used index for g^- (group scattered into)
ILIST	Local EVXS,ADREAD	Trigger to omit prints used for debugging
ILR	Blank Common	Block of lengths of output required for given reaction
IMAX	Blank Common	ECS requested on JOB CARD
IMD	Local DATEC	Origin in AA block for MD block for call to COEF
IMG	Local DATEC	Origin in AA block for MG block for call to COEF
IN	Blank Common	Origin in AA block for 10 input parametera for current material (SID)
INC	Local PRTGG,FINIS	Increment for printing

TABLE XII (Cont.)

Name	Storage location	Definition
INDTC	Local PUNCL	Indicator of type of output required
INDTH	Local PUNREP	Indicator of number of digits to use in numbering card output: 0 = three; 1 = two
INIT	Local SSS	Pointer to AA block for output prints
INP	Local EVXS	Total number of sets of input data allowed in one run ($\leq$ 20)
IOUT	Blank Common	Initial position in ECS for storing output
IP	Blank Common	Number of input parameters stored on ECS for each material (currently 10)
IPAR	Blank Common	Temporary block for switching parameter sets
IPH	Local DATEC	Origin in AA block for PH block for call to COEF
IPN	Local EVXS,FINIS	Input parameter: 0 = Transport correction for output; 1 = Consistent PN
IPOE	Local DATEC	Origin in AA block for POE block for call to COEF
IPR	Local ERROR	Indicator of type of error and action to be taken
IR	Blank Common	Index for reaction currently being processed (IR = 1,..., R)
IRDCT	Local PUNREP	Storage blocks (6 for each card) for number of repeats for each field
IRDNUM	Local PUNREP	Storage block for value from each field
IRDOP	Local PUNREP	Storage block for operation to be applied to value in field
IREM	Local SSS	Number left to print
IRS	Blank Common	Length of blocks of data (ESJ) for "laws" for each reaction ($\leq$ 3000)
IS	Blank Common	Lengths of cross-section blocks (SIG) for each reaction ($\leq$ 3000)
ISAV	Local SSS	Pointer to AA block for printing
ISC	Local DATEC	Origin in AA block for SC block for call to FINIS
ISF	Local DATEC	Origin in AA block for SF block for call to FINIS
ISG	Local DATEC	Origin in AA block for SIG block for call COEF
ISIG	Blank Common	Block of origins in ECS for SIG and ESJ blocks for each reaction
ISO	Local EVXS,FINIS	Input parameter for degree of anisotropy ($\leq$ NMAX)
ISR	Local EVXS,DATEC	Sum of lengths (for ECS) of SIG and ESJ blocks for all reactions $= \sum_r (IS_r + IRS_r)$
ISS	Local DATEC,FINIS	Origin of output block in AA block (SS)
ISTO	Local DATEC	Origin in AA block for STO block for call to FINIS
IST1	Local DATEC	Origin in AA block for ST1 for call to FINIS
ITAP	Blank Common	Scratch tape (=3)
ITB	Local NEWPG,FINIS	Number of the table being printed
ITBL	Local MAIN, FINIS	Input parameter for ITL < (G + 3): 0 = Floor output cross sections; 1 = Truncate
ITID	Blank Common	Block of origins in ECS for angular distributions
ITK	Local DATEC	Origin in AA block for TK block for COEF

TABLE XII (Cont.)

Name	Storage Location	Definition
ITL	Local EVXS,FINIS, CARDS	Input parameter for output table length desired (if < 0, print only)
ITYPE	Local PUNREP	Type of output format to use: -1 = ANISN, 0 = DTF (end with 3), +1 = DTF (end with 9)
IT1	Local COEF,FTBLN, FISSN	Integer value to test for ESJ pointer, -1.0, to indicate end of sublists and/or end of block
IT2	Local FTBLN	Integer value to test for ESJ pointer, -2.0, to indicate end of sublists
IT4	Local FTBLN,LAWFR, NUMBR	Integer value to test for ESJ pointer, -4.0 to indicate end of sublists
IT5	Local FTBLN,NUMBR	Integer value to test for ESJ pointer, -5.0, to indicate end of sublists
IVECP	Local PUNREP	Vector containing data to be processed
IWRT	Local SSS	Pointer to first number to be written
IW4	Local EVXS,FINIS	Input parameter for type of output desired
IX	Local EVXS,DATEC	Total ECS storage required for output
	Local DATEC	Origin of X block in AA block for call to COEF
	Local FTBLN,NUMBR, PRTGG,FINIS	Temporary index
IXS	Blank Common	Type of storage required for output for a given reaction
IZ	Blank Common	Indicator for gamma deposition calculation if > 0: 1 = Save storage 2 = Print header 3 = Calculation for one reaction 4 = Final calculation for one material
I1	Local EVXS,GREAD, GPOE,COEF,FINIS	Index for E_g- from block EK
I2	Local EVXS,GREAD, GPOE,COEF,FINIS	Index for E_g+ from block EK
I24	Blank Common	Data for unpacking indices from blocks MG, ME, MD (= octal 10^8)
I3	Blank Common	Count of number of times FTBLN has been entered, initially zero
I4,I5,I6	Blank Common	Counters for Laws 2, 5, and 6, respectively
I8	Local COEF,TINEL	If nonzero, indicates angular distribution for nonelastic reaction
JD	INT Common	Index for current value of angular distribution energy (E(JD))
JEC	Local EVXS,DATEC	Current origin in ECS to read data
JF	Local COEF,FISSN	Pointer for the ν block for fission reaction
JG	INT Common	Index for current value of cross-section energy (ES(JG))
JX	INT Common	Index for current value of cross-section energy (ES(JX))
J1	INT Common	Index for initial value in TK and ESJ blocks
J2	INT Common	Index for final values in TK block
J3	Local COEF	Initial value of JX, position of first nonzero SIG in table
KF	Blank Common	Input parameter for type of Chi handling: 0 = normal; 1 = like MANIAC code; 2 = print matrix before summing

TABLE XII (Cont.)

Name	Storage Location	Definition
KG	Blank Common	Number of flux (PH) and energy (EK) values for group set G1D ($\leq$ 500)
KH	Local NEWPG	Temporary indicator of type of output desired
KJ	Blank Common	Current value of IRS_r, length of ESJ block for reaction being computed
KM	Local NEWPG	Number of tables being computed
KT	Blank Common	Number of words in angular distribution block TK
K2	Blank Common	Number of data to describe energy distribution of outcoming neutrons (not used in EVXS)
LA	Blank Common	Length of storage in AA block needed for given material
LAST	Local SSS	Pointer for final number to write
LAT	Local DATEC,FINIS	Temporary word for length of AA block
LDIF	Local REORDR	Difference between last nonzero cross section and largest energy
LEFT	Local CARDS	Number of remaining values less than enough to fill a card
LEG LEGN	Blank Common INT Common	Number of Legendre coefficients used: 0 = none, n = NED
LEN	Local FINIS,CARDS	Temporary word for gamma energy deposition calculation (= G * ITL)
LGID	Blank Common	Length of block stored for each group set (G1D) (= G + 2 * KG)
LIS	Blank Common	Storage required in AA block for longest ESJ_r ($=IRS_r$)
LLG	Local EVXS,DATEC, PRTGG	Value to use in computing storage needed for output (= IGP * G * NAX)
LTAP	Blank Common	Scratch tape (= 4)
LTID	Blank Common	Storage required in ECS for given angular distribution (= KT + 2 * NED)
LTOT	Local EVXS,ADREAD	Total ECS storage required for given material
LWRT	Local SSS	Pointer to last word to be written from AA block
LW1	Local SSS	Index for LWRT
L10	Blank Common	Counter for Law 10
MD	Local ADREAD,COEF TININ	Packed indices to the TK block corresponding to energies in the E block
ME	Blank Common	Packed indices to ES block for which nonzero cross sections (SIG) are given for each reaction
MG	Local GREAD,GPOE COEF	Packed indices for KG block indicating energy bounds
MIX	Blank Common	Indicator of type of material: 0 = Isotope, 1 = Mixture (not used in EVXS)
MSR	MSG Common	Block containing description of reaction for each ID for output printa
MTAP	Blank Common	Variable name for output file (=2)
NAX	Blank Common	Temporary storage for current maximum P_n (NMAX(NM))
NCARD	Local PUNREP	Number of entries per card
NCHCVT	Local PUNREP	Number of characters to convert
ND	Blank Common	Number of angular distributions for current material
NEC	Blank Common	Current initial position in ECS into which input data is to be stored
NED	Blank Common	Number of energies for which angular distributions are given ($\leq$ 400)
NEN	Local PRTGG	Current count of ECS required for output of computed values

TABLE XII (Cont.)

Name	Storage Location	Definition
NES	Blank Common	Number of energies in ES block ($\leq$ 3000)
NF	Local TE,FINIS	Number of functions in TK block for $P_n(\mu_L)$
NG	Blank Common	Number of sets of group data to be used ($\leq$ 10)
NINC	Blank Common	Number of subdivisions to use in du integral (usually 40)
NINP	Local COEF,FTBLN	= NINC + 1
NM	Blank Common	Index of material procesaing loop
NMAX	Blank Common	Block of values of maximum P_n to use for material being evaluated ($\leq$ 10)
NN	Blank Common	Index n for P_n
NOENC	Local PUNCL	Current number of entries
NOENR	Local PUNCL	Number of entries remaining
NOENT	Local PUNCL	Number of entries per card
NOINP	Local PUNCL	Number of single characters for input
NOMEC	Local PUNCL	Count of characters being moved
NOSSCCH	Local PUNCL	Number of single characters to change
NOTLP	Local PUNCL	Scratch file
NOUT	Local PUNREP,PUNCL	Variable name of output file
NP	Local EVXS,TININ	Index for processing loop for all materials
NPN	Blank Common	Temporary storage for IPN for current material
NR	Local PRTGG,FINIS, PRTB	Number of values remaining to be printed
NREMOD	Local PUNCL	Number of single characters for output
NS	Blank Common	Number of material sets in library
NSID	Local FINIS	Origin of output parameter block
NSTART	Blank Common	Initial ECS position for storing cross-section data upon starting new material
NT	Blank Common	Number of materials to be evaluated ($\leq$ 10)
NTAP	Blank Common	File containing data library (= 1)
NTAPE	Local PUNCL,PUNREP	Indicator of output media desired: 0 = punched cards, N = magnetic, decimal tape N
NTAPET	Local PUNREP	Scratch file
NZ	Blank Common	Z-number for material
PE	Local COEF	= EDL * ED
PH	Local GREAD,GPOE, COEF	Block of values for flux-weighting corresponding to energy values in EK block
PL	Local COEF,TININ	Block of temporary functions for nonelastic angular distributions
POE	Local GPOE,COEF	For ϕ (E) dF, $POE = P_1 = \ell n\ (PH_k) - X_1\ \ell n\ (EK_k)$
PS	Local COEF,SSUM	= POE (JG) + SOE (+ ZOE if fission reaction)
Q	Blank Common	Value of QR_r for current reaction
QR	Blank Common	Block of energies released for each reaction ($\leq$ 50)
R	Blank Common	Number of reactions for given material ($\leq$ 50)
RQ	INT Common	Absolute value of Q for current reaction
R1	INT Common	$= 1.0 + AM^2$
R2	INT Common	= 2 * AM
R3	INT Common	= AM

TABLE XII (Cont.)

Name	Storage Location	Definition
S	Local TE	Temporary storage while summing to NF for: $2 * T(\mu,E_i) = 1 + \sum_{n=1}^{NF} (2n+1) * F_n * P_n(\mu)$
SC	Local FINIS	Block in which final DTF format cross sections are stored
SDES	Blank Common	Description of material requested
SE	Local COEF	Difference between two consecutive angular distribution energies (ED - EDL)
SF	Local FINIS	Storage block for nu-sigma fission$_g$ ($\nu\sigma_g f$)
SID	Blank Common	Ident number of material requested (= SIDN(NM))
SIDN	Blank Common	Block of material idents (SID) to be processed ($\leq$ 10)
SIG	Local SGREAD,REORDR, COEF,SPACE, GSOE	Block of cross-section data values cotresponding to energies in the ES block ($\leq$ 3000)
SIN	Local EVXS,DATEC	Temporary storage for current SID
SOE	INT Common	For $\sigma_r(E_i)$, SOE = S_i = $\ell n(\sigma_j)$ - Y * $\ell n(E_j)$
SS	Local(Many)	Block into which output for each reaction is stored as computed before writing on ECS
STO	Local FINIS	Cross-section block storage for even k-table
ST1	Local FINIS	Cross-section block storage for odd k-table
SUM	Local COEF,INTG	Temporary storage for summing an integral
SY SYS	Blank Common INT Common	Syatem used in calculation: 1 = center-of-mass; 2 = lab system
S1	Local COEF,FTBLN, MAY,PRTGG	Block of Chi's by group for fission reactions (χ_g)
S2	Local COEF,PRTGG	Block of $\nu\sigma_g^f$ for fission reactions
S10	Local NUMBR	Temporary storage for $\frac{E2 + E1}{2}$
TAD	Local MAIN	Block into which title and description of current version of library are read
TDES	Blank Common	Description block for current angular distribution
TID	Blank Common	Identification number for current angular distribution (= $TIDR_r$)
TIDR	Blank Common	Ident numbers of angular distribution to be used with rth reaction (none if < 0)
TIDS	Blank Common	Ident numbers of angular distributions in order found in library for given material ($\leq$ 25)
TK	Local ADREAD,COEF, INTG,TE,TININ	Block of angular distribution data ($\leq$ 4000)
TM	Local COEF,INTG, GETHU	μ_{min} in elastic and discrete inelastic calculation
TMP	Local FTBLN,LAWFR, FINIS	Absolute value of difference between weight and integral
TOL	Blank Common	Value to determine step size in integrating nonelastic
TOT	Local COEF,PRTGG	Temporary storage for total scattering cross section for given reaction
TP	Local COEF,GETHU	μ_{max} in elastic and discrete inelastic calculatica
TYPE	Blank Common	Type of reaction being processed (= TYPER(ID))
TYPER	MSG Common	Block of type numbers corresponding to ID number for each reaction

TABLE XII (Cont.)

Name	Storage Location	Definition
U	Local INTG,TE,PN,FF	Temporary value of cosine in computing angular distribution
UB	Local COEF,TININ, TINEL	Angular distribution functions for nonelastic computation
UL,UM, U1,U2	Local INTG	Temporary storage for μ values when picking up intermediate points where data are given (normal step size is 1/40 of distance from -1.0 to +1.0)
VECP	Local PUNCL	Block of data to be processed
W	Local FTBLN,LAWER, NUMBR	Weight factor from ESJ block
WT	Local FINIS	Weight currently being used
WT4	Local FINIS	Special weight function (=0.6023/A) for TD4
X	Local GPOE,COEF	Block of values for X_i ($=\ell n(\phi_{k+1}/\phi_k)/\ell n(E_{k+1}/E_k)$)
XSUM	CMPUTE Common	Integral for g or g'
XY	Local COEF,SSUM	= X(JG) + Y (+Z if fission reaction)
Y	INT Common	Current value of: $= \ell n(\sigma_{j+1}/\sigma_j)/\ell n(E_{j+1}/E_j)$
Z	Local COEF,FISSN	Current value of: $= \ell n(\nu_{i+1}/\nu_i)/\ell n(E_{i+1}/E_i)$
ZOE	Local COEF,FISSN	For fission reaction = $\ell n(\nu_i)$ - Z * $\ell n(E_i)$

V. CODE OPERATION

At this time the program and the LAMDF are stored together on a magnetic tape in binary format, the code as an UPDATE[10] OLDPL in the first file and the data on the following NS files as described in Sec. II.A. Ultimately, we hope to have both the program and the library permanently stored on disk.

The FORTRAN code is prepared for execution by making an UPDATE run in which a BCD card image file is written to the COMPILE file which, in turn, is input to the compiler. The UPDATE program allows convenient modification of the current version of the code, but if sufficient use is made of the code and modifications are not generally required, a compiled binary version could be stored either on disk, on the tape in place of the OLDPL, or on the tape as an additional file preceding the OLDPL. In this section we summarize the input and output options available in EVXS.

A. Input

The data deck required to obtain cross sections for one or more materials in the LAMDF consists of the following cards:

(1) Title card - Contains descriptive data supplied by the user to identify the particular run (8A10 format).

(2) Parameter Cards - Contain control parameters, one card for each material for which cross sections are desired. The details are given in Table XIII. The first three parameters are required for each material, while the rest are optional, with defaults as shown in the table (12I6 format).

(3) Blank Card - Signifies the end of the parameter cards.

TABLE XIII

INPUT PARAMETERS FOR EVXS

Parameter Name	End in Column	Description	Default
GIDN	6	N = Group set to be used (if GIDN < 0, group structure information must follow the blank card as described in text)	None
SIDN	12	N = Identification of cross section to be processed	None
NMAX	18	N = Number of P_n components to be calculated. See restrictions discussed in Sec. III.E below Eqs. (121b), (122b), and (123b)	None
ITL	24	N = Output table length desired (if list only is desired, set negative)	G + 3
IHT	30	N = Position in table of total cross section	3
IHS	36	N = Position in table of self-scatter cross section[a]	4
ISO	42	N = Degree of anisotropy	1
IPN	48	0/1 = Transport correction/consistent P_n (see Sec. III.E)	0
ITBL	54	0/1 = Floor/truncate output[b]	0
IW4	60	N = Special output option[c]	0
IK	66	0/1 = K-Table only (K = ISO)/all tables, K = 1,..., ISO	0
KF	72	0/1/2 = Fission matrix handling: normal/like MANIAC code/matrix printed (see Sec. III.E, Eqs. (117) and (118)	0

[a] Space can be allowed for upscatter terms between IHT and IHS and for other special terms at the beginning of the table as shown in Table VIII.

[b] ITBL indicates how scattering beyond limits imposed by table length will be handled: Floored - Scattering is not permitted below the lowest energy group allowed by table length and is added to next higher group "up the diagonal" (method used by the MANIAC code). Truncated - Scattering below the lowest energy group is added into the absorption cross section to maintain the neutron balance (see Sec. III.E, especially Eqs. (124) and (125)).

[c] Depending on values of IW4, the following output options are available:
0 = Old DTF output
1 = TD4 version of output
2 = Gamma energy deposition calculation
3 = Output for the ANISN loader
4 = Output for the DTF loader, blocks terminate (end with 3)
5 = Output for the DTF loader, blocks continue (end with 9)

In general, group sets and materials can be paired in any fashion desired, with the same group set used for some of the materials or the same material being used with different group sets or different input parameters. No particular order is required of the input material requests since they are sorted and will be calculated in the order in which they are found in the library. A special exception is the Gamma Disposition Calculation input which will be described. More than one group of requests can be included in one run by separating the groups by blank cards and omitting the title card after the first set. The library will be rewound and the second set processed. A Gamma Deposition Calculation could be run here.

When group set data are to be added from the input stream rather than taken from among those existing in the LAMDF, the parameter GIDN is set to -GID and the set of cards is added directly behind the blank card which ends the set of cross-section requests. The required format for the group sets is given in Table XIV.

The special option for nonfission neutron and gamma energy deposition calculations is described in Sec. III.F. To make such calculations, IW4 must be set to 2 and IPN to 1. The trigger IW4 = 2 need be set on only one of the parameter cards. The same group set (GID) must be used for all materials in one run for this special option. The materials must be requested in the same order in which they are available in the LAMDF; this is an exception to the general rule. Other input data required are the gamma energy production cross sections for each group for each material requested in the parameter cards. These additional cards follow the blank card; however, if the GID group set is read in on cards, then the special cards follow the group set cards. For each material we put in a title card (8A10 format) and as many cards as are needed for the gamma energy production cross sections GI_g, g = 1,...,G in 6E12.5 format. The index g here runs from the lowest to the highest energy group. It may be helpful to review the overall input card structure for the gamma energy deposition option:

(1) Title card for the run.

(2) Data cards for all materials desired with the same GID on each card; NMAX = 1, IPN = 1, and IW4 = 2.

(3) Blank card.

(4) Gamma energy production cross sections in MeV-barns for all materials, in the same order as the materials are requested above, each set of cross sections preceded by a title card.

TABLE XIV

GROUP SET CARD FORMAT

Card Block	Length	Format	Contents
1	1 card	(3I6,6A10)	GID, G, KG, Comment (60 BCD characters)
2	G values	(12I6)	MG block, indices for the PH and EK blocks
3	G values	(6E12.4)	GE block, group energies[a] in MeV
4	KG values	(6E12.4)	PH block, weighting fluxes in MeV^{-1}
5	KG values	(6E12.4)	EK block, energies in MeV at which fluxes are given

[a]These quantities are used only in SUBROUTINE SSS; if there is to be no Gamma Energy Deposition calculation, any values, including 0.0, can be used here.

B. Output

The options for card or tape output from EVXS are:

If ITL < 0 the cross sections are listed only on the output file.

If ITL > 0, the cross sections are listed on the output file and written in BCD card image format on unit LTAP = 4. The specific format depends on the value of IW4.

If IW4 = 0, the BCD card images are in standard DTF format.

If IW4 = 3, the BCD card images are in DTF format acceptable to the ANISN loader.

If IW4 = 4, the BCD card images are in DTF format appropriate for the DTF loader with data blocks ending with termination character 3.

If IW4 = 5, the BCD card images are in DTF format appropriate for the DTF loader with data blocks ending with continuation character 9.

The BCD card images on unit LTAP may be punched using the PUNCHIT control card or else by assigning TAPE 4 to PUNCH in the PROGRAM card.

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