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RESEARCH ESTABLISHMENT
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by

E.K. ROSE

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ABSTRACT

This report is a guide to the contents and layout of the A.A.E.C. fission product point cross section library FISPROD.POINTXSL and the group cross section library FISPROD.GROUPXSL, and to the IBM 360/50 FORTRAN IV programs associated with the generation and subsequent updating of these two data libraries.

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CONTENTS

1. INTRODUCTION

A point cross section library (FISPROD.POINTXSL) has been prepared for 192 fission products (184 ground states plus 8 isomeric states) in the layout and format of the U.K.A.E.A. Nuclear Data Library (Parker 1963). The group cross section library FISPROD.GROUPXSL was created from this point data library using a group averaging program to produce group data in the 127-group structure of GYMEA (Pollard and Robinson 1966). Both libraries are currently available on magnetic tape.

The total energy range covered by the libraries is 10^{-9} MeV to 15 MeV, with the original point cross section data drawn from three separate sources. The eV region is from Ferguson's (1969) cross section generating code GUNYA, the keV region from Musgrove's (1969) theory, and the MeV region from a combination of Bertram's (1969) COMPOST results and Benzi and Reffo's (1969) $\sigma_{n\gamma}$ values.

The three programs associated with the point cross section library generation and updating are:

(i) the initial data processing program LOAD which creates separate data files on disk for each region,

(ii) the point cross section generating program FPLGP which uses these three data files, and

(iii) the editing and updating program FPEDIT.

The programs associated with the group library are:

(i) the group averaging code BOMB (Doherty 1969) and

(ii) the editing and updating program GPEDIT.

2. DESCRIPTION OF THE LIBRARIES

2.1 The Point Data Library FISPROD.POINTXSL

2.1.1 Description

Following the layout of the U.K.A.E.A. Nuclear Data Library, each nuclide is associated with a three-digit nuclide identification number NIN (for example NIN = 1 for ^{72}Zn, 184 for ^{165}Ho). The cross section data are classified by a five-digit reaction type number RTN which is sub-divided into a two-digit general classification number GCN followed by a three-digit particular classification number PCN. GCN = 1 for neutron cross section data, and PCN = 001, 002, 003, 004, 102, 201 respectively for the total, elastic, non-elastic, (n, n'), (n,γ) and transport reactions, these six reactions only being required for the point data library.

The library consists of a preface section which identifies each nuclide with its corresponding NIN and the total number (NC) of 80-byte records for that nuclide, followed by NNUC data blocks, one per nuclide, in the order stated in the preface section. Each individual nuclide data block consists of Section 00, followed by 6 sections, one per reaction, in ascending order of PCN, containing the energy-cross section values for the energy range $10^{-9} \leqslant E \leqslant 15$ MeV.

2.1.2 Contents and format of data sections

All records, being EBCDIC card images, are 80 bytes in length, blocked to 7280 bytes (blocking factor = 91).

Preface section

Record 1 contains NNUC, the total number of fission products available in the library in format (I11) .

Records 2 to (NNUC + 1) contain, in format [3(I11,1X)] , the quantities NIN, NC, NUCLAB, per nuclide,

with NIN and NC as defined in Section 2.1.1 and

NUCLAB = label for each nuclide

= symbol + atomic mass number (e.g. ZN072).

Section 00 in format [6(I11,1X),I3,I2,I3]

Each record contains 6 data items plus labelling in bytes 73–80.

Record 1: Item 1 = NIN

2 = NC

3 = NS = number of records in Section 00

4 = atomic number Z (fixed point)

5 = atomic mass A (floating point)

6 = number of different reaction types = 6

Records 2 to (NS–1):

Item 1, 4 etc. = section number (1 to 6)

2, 5 etc. = reaction type number (1001, 1002, 1003, 1004, 1102, 1201)

3, 6 etc. = number N_i of records in this section (i = 1 to 6).

For labelling in bytes 73–80 see below.

Sections 1 to 6 (cross section data)

Record 1: Item 1 = RTN (e.g. 1001)

2 = number of energy ranges = 1

3 = 'Q' value of reaction in MeV = 0

4, 5, 6 are blank for this library.

bytes 73–75 = NIN

76–77 = Section number

78–80 = Serial number

Record 2: Item 1 = lower limit of energy range = 1.0252×10^{-9} MeV

2 = upper limit of energy range = 15 MeV

3 = material temperature = 0° A

4 = number of cards in data file = $N_i - 1$

5 = number of cross section points = NX

6 = number of temperatures to be considered = 1 for this library.

The (N_i-2) records which follow contain NX pairs of energy-cross section values (3 per record) plus labelling in bytes 73–80 per record. Section 00 and Sections 1 to 6 are repeated for each of the NNUC nuclides, the completed library being closed by an end-of-file mark.

2.1.3 Cross section data sources

The three data files FISPROD.EVREG, FISPROD.KEVREG and FISPROD.MEVREG were created by program LOAD, whereas all adjustments and calculations of further cross section data were performed by the main program FPLGP.

eV Region data

The source of the eV region data was the neutron cross section generating code GUNYA (Ferguson 1969) which produced 127 group cross sections for the (n,γ) and transport reactions over the energy range E = 10 MeV down to $E \sim 10^{-9}$ MeV for the 192 fission products in the library. The output from GUNYA preceded by an 80-byte title record and the 128-group energy boundaries (in descending order) constitutes the eV region data file FISPROD.EVREG currently on disk pack 5.

As the required eV region data set covers the resolved resonance region only, the GUNYA energy range was truncated at the energy boundary just below 5 keV (E_ℓ = 4.3117 keV) for all nuclides except those with resonances resolved above this energy. There are only nine nuclides in the set of 192 fission products with the last resolved resonance energy $E_R > 5$ keV. For these nuclides E_ℓ was selected as the nearest upper energy boundary to E_R.

The group cross section values were converted to point values by representing each group by two points at energies straddling each boundary. By this means the group cross section in group $(E_j \rightarrow E_{j+1})$ was represented by the 2 points $(E_j + dE_j, \sigma_j)$ and $(E_{j+1} - dE_{j+1}, \sigma_j)$, where $dE_j = duE_j$ with du = 0.001, and hence any subsequent group averaging process will reproduce the original group data.

The six reactions in the library are σ_{total}, $\sigma_{elastic}$, $\sigma_{non\text{-}elastic}$, $\sigma_{nn'}$, $\sigma_{n\gamma}$, and $\sigma_{transport}$. Given $\sigma_{n\gamma}$ and $\sigma_{transport}$, the remaining cross sections can be evaluated from the formulae:

$$\sigma_{total} = \sigma_{elastic} + \sigma_{non\text{-}elastic}$$

$$\sigma_{transport} = \sigma_{elastic}\left(1 - \frac{2}{3A}\right) + \sigma_{non\text{-}elastic}$$

$$\sigma_{non\text{-}elastic} = \sigma_{n\gamma} + \sigma_{nn'}$$

and $\sigma_{nn'}$ is set to 0.0

(A = atomic mass of nuclide) .

keV Region data

The keV region data was produced by a program which incorporated the cross section generating theory of Musgrove (1969). The $\sigma_{n\gamma}$ and σ_{total} values (in millibarns) thus obtained for the 192 fission products over the energy range 5–100 keV have been placed onto data file FISPROD.KEVREG on disk pack 5.

The keV region extends from $E_\ell \sim 5$ keV to 100 keV. The remaining cross sections were again calculated from the above formulae.

MeV Region data

The point data compiled for the MeV region (0.5 MeV to 15 MeV) is a combination of data ($\sigma_{elastic}$, $\sigma_{nn'}$, σ_{total},) derived from Bertram's (1969) program COMPOST and $\sigma_{n\gamma}$ values from the report by Benzi and Reffo (1969). The data file FISPROD.MEVREG on disk pack 5 was created from these two sources.

To ensure continuity of $\sigma_{n\gamma}$ at 100 keV and preserve the shape of the MeV region $\sigma_{n\gamma}$ contour, the Benzi and Reffo data were normalised for each nuclide to the 100 keV value of FISPROD. KEVREG, and the total cross sections corrected by the addition of the adjusted $\sigma_{n\gamma}$ values. The values of $\sigma_{transport}$ and $\sigma_{non\text{-}elastic}$ were calculated from the above formulae.

2.2 The Group Data Library FISPROD.GROUPXSL

2.2.1 Description

Following the convention used for the point cross section library FISPROD.POINTXSL, each nuclide is identified by its nuclide identification number NIN and each cross section by its reaction type number RTN. The group cross section values were calculated by program BOMB (Doherty 1969) which group-averages the point data of FISPROD.POINTXSL over the 127-group structure of GYMEA. The group library contains 6 reactions for each of the 192 nuclides in the same order as the point cross section library.

2.2.2 Contents and format of library

Again all records, being EBCDIC card images, are 80 bytes long, blocked to 7280. The first two records contain the library name FISPROD.GROUPXSL (bytes 1–16) and some identification comments. The next 22 records contain the 128-group lethargy boundaries (0 to 23) in ascending order [format (6E12.5)]. Then follow 192 data blocks, one per nuclide, consisting of the following information per block;

(i) nuclide identification label
NIN, NUC, IA
in format (9X,I3,A2,I3),
where NIN = nuclide identification number,
NUC = chemical symbol,
IA = atomic mass number,

(ii) cross section identification number
RTN, in format (10XI4),

(iii) 22 records for the 127 group cross section values, 6 per record, in format (6E12.5), for the reaction specified by the above RTN, with the highest energy value first, and

(iv) a terminator record for each reaction containing in bytes 1 → 80
*b$$$ .....$
where b denotes a blank, and $ a dollar sign.

Items (ii) to (iv) are repeated for each of the 6 reactions in ascending order of RTN, each nuclide block being terminated by a record with *b** .....* in bytes 1 → 80. The complete library is closed by an end-of-file mark.

3. PROGRAMS LOAD, FPLGP, FPEDIT ASSOCIATED WITH FISPROD.POINTXSL

3.1 The Program LOAD – Initial Data Loading Program

3.1.1 Description

LOAD was written to create data files FISPROD.EVREG, FISPROD.KEVREG, FISPROD.MEVREG on disk pack 5 from the original cross section data available either on disk as in the case of the GUNYA output on FISPROD.GUNYA, or from cards as for the keV and MeV region data obtained respectively from Musgrove's theory and COMPOST (combined with the Benzi and Reffo $\sigma_{n\gamma}$ values). A counter ℓ (1 → 5) allows the generation of any one of these files, or combinations thereof, at any one time. A separate file FISPROD.COMPOST was created for the COMPOST data as a back-up copy, and also to facilitate the addition of updated $\sigma_{n\gamma}$ values at some later date.

3.1.2 Operating instructions

Input to LOAD

Card 1 contains L, TITLE

where L, in column 1, is a counter specifying the data file to be created during this run, and TITLE (columns 3 → 78) is any required heading for the PRINTER output. L is set to:

1 for the creation of FISPROD.EVREG on FT unit 10 from energy values on cards and from GUNYA cross section data on FT unit 8,

2 for the creation of FISPROD.KEVREG on FT unit 11 from data on cards,

3 for the creation of FISPROD.COMPOST on FT unit 12 from card input,

4 for the creation of FISPROD.MEVREG on FT unit 13 from FISPROD.COMPOST data set on FT unit 12 plus the Benzi and Reffo $\sigma_{n\gamma}$ values on cards; this allows updating of $\sigma_{n\gamma}$ values at some later date,

5 for the creation of both FISPROD.COMPOST on FT unit 12 and FISPROD.MEVREG on FT unit 13 both from initial card input.

L = 1 The creation of FISPROD.EVREG requires the additional card input 22 cards containing the 128-group energy boundary values (in units of eV in descending order) in format (6E12.5).

The $\sigma_{n\gamma}$, $\sigma_{transport}$ data sets for each of the 192 nuclides are provided by FISPROD.GUNYA which is the output file from the GUNYA code.

L = 2 The creation of FISPROD.KEVREG requires the following additional card input for each nuclide;

(i) card containing ØØNUCLIDEØ,LABEL,A in format (10X, A2,I3) where the first 10 columns are optional, LABEL = nuclide symbol (e.g. ZN), A = atomic mass number (integer),

(ii) set of energy-cross section values E, $\sigma_{n\gamma}$, σ_{total} per card in format (8XI3,32X2E10.2) for 5 keV ⩽ E ⩽ 100 keV.

192 sets of (i) and (ii) completes the input to this problem.

L = 3 The creation of FISPROD.COMPOST requires the additional set of cards containing Z, A, E, $\sigma_{elastic}$, $\sigma_{nn'}$, σ_{total} in format (6F8.3) for 0.5 MeV ⩽ E ⩽ 15 MeV.

L = 4 The creation of FISPROD.MEVREG requires FISPROD.COMPOST on disk (unit 12) plus additional card input per nuclide;

(i) card containing (LABEL, A) in format (1X,A2,I3) where LABEL = nuclide symbol, A = atomic mass number,

followed by

(ii) the $\sigma_{n\gamma}$ values at the same energy points as the COMPOST data set (0.5 MeV ⩽ E ⩽ 15 MeV) in format (8E10.3), with the 0.1 MeV value as the first number on the card.

L = 5 is merely a combination of L = 3 and L = 4 and requires card data in that order.

Output from LOAD

LOAD creates labelled data files on disk pack 5 (with a copy listing on the PRINTER) in the following layout and format. All records are 80 bytes in length and blocked to 7280.

FISPROD.EVREG

Record 1:	heading of file in format (20A4)
Records 2 →23:	E_i (in eV), i = 1 → 128 in format (6E12.5)
	with $E_1 = 10^7$ eV
	$E_{128} = 1.0252 \times 10^{-3}$ eV
Record 24:	**NNnnn (N,GAMMA) (columns 1 onwards)
where	NN = nuclide symbol
	nnn = atomic mass number (e.g. ZNb72)
Records 25 → 46:	127 group values of $\sigma_{n\gamma}$ in format (6E12.5)
Record 47:	**NNnnn(N, TRANSPORT)
Records 48 → 69:	127 group values of $\sigma_{transport}$ in format (6E12.5).

The layout and format of records 24 to 69 are repeated for the 192 fission products in the order of the library. An end-of-file mark terminates this data file.

FISPROD.KEVREG

Record 1:	heading for file in format (20A4)
Record 2:	bbNUCLIDEbNNnnn (in columns 1 onwards)
Records 3→22:	in format (8XI3,32X2E10.2) [= original card image]
	contain E(keV), $\sigma_{n\gamma}$(mb), σ_{total} (mb) per record for E=5(5)100 keV.

Records 3 → 22 are repeated for each of the 192 nuclides in the library, the file being closed by an end-of-file mark.

FISPROD.MEVREG

Record 1:	heading for file in format (20A4)
Record 2:	Z, A, 0.1, $\sigma_{n\gamma}$ (at 0.1 MeV)
Records 3 →13:	Z, A, E_i, $\sigma_{n\gamma_i}$, $\sigma_{e\ell_i}$, $\sigma_{nn'_i}$, σ_{total_i}
	i = 1 → 11, $0.5 \leqslant E_{i1} \leqslant 15$ MeV, in format [3F8.3,F8.5,3F8.3]

Records 2 →13 are repeated for all 192 nuclides, the file terminating with an end-of-file mark.

FISPROD.COMPOST is similar in layout to FISPROD.MEVREG except that record 2 is omitted and the contents of the remaining records are:

Z, A, E_i, $\sigma_{e\ell_i}$, $\sigma_{nn'_i}$, σ_{total_i} per record in format (6F8.3) for $0.5 \leqslant E \leqslant 15$ MeV.

3.2 The Library Generating Program FPLGP

3.2.1 Description

Using data source files FISPROD.EVREG, FISPROD.KEVREG and FISPROD.MEVREG on FT units 10, 11, 12 respectively, program FPLGP manipulates these data sets, generating cross section data for 6 reactions over one continuous energy range (.001 eV $\leqslant$ E $\leqslant$ 15 MeV). From the eV region data the subroutine EVREG first determines the cut-off energy E_ℓ, then calculates the missing reactions and finally represents each GUNYA group cross section by two points (see 2.1.3). This expanded data set is dumped on temporary FT unit 4. Subroutine KEVREG handles the keV region data, temporarily dumping it on FT unit 5; while subroutine MEVREG normalises the $\sigma_{n\gamma}$ values, adjusts the total cross section and puts the 6 required reactions onto FT unit 7. The three correct point data sets on FT units 4, 5 and 7 are then merged for each reaction and nuclide by subroutine TOTREG and dumped onto FT unit 8. Lastly subroutine CREATE creates the U.K.A.E.A. type fission product point cross section library FISPROD.POINTXSL on FT unit NUT (specified by user)

from the data available on FT unit 8. The library may be generated in sections (i.e. any number of nuclides per run) provided a sequential order of nuclides, starting with NIN = 1, is observed.

3.2.2 Operating instructions

Input to FPLGP

Card input (one card only)

NUT, NFILE, NP1, NP2, DATE in format [4I3,1X2A4]

where NUT = FT unit number of output device (say 13 or ⩾ 15)
= blank for PRINTER only

NFILE = number of nuclides already created, at some previous date, on the output unit specified above
= blank for initial creation of library

NP1, NP2 = first and last nuclides (per NIN) to be generated.

DATE = date: xx/xx/xx

Disk input

The cross section data must be available from data files FISPROD.EVREG, FISPROD.KEVREG, FISPROD.MEVREG on FT units 10, 11, 12 on disk pack 5. Temporary working space must be allocated for FT units 4, 5, 7, 8 and 14.

Output from FPLGP

FPLGP creates the fission product point cross section library FISPROD.POINTXSL on the output device specified by FT unit NUT in the layout and format described in Section 2.1.2. A printer listing is obtained at the same time. When creating the library in sections, only the output for those nuclides whose cross section data are being generated during the run, is made available on the printer, each new set being preceded by the 'preface section' with updated NC values.

3.3 The Editing and Updating Program FPEDIT

3.3.1 Description

The program FPEDIT was written to provide an editing and updating facility for the fission product point cross section library once it has been generated on tape. Three options and certain combinations are available;

(i) listing and/or copying of any nuclide data set in the library,

(ii) updating of any cross section block from new data on cards, and

(iii) plotting of (σ vs E) graphs on log-log scale for any cross section set.

A counter ℓ (0 →5) is used to specify the three fundamental options and their combinations, (see 3.3.2). The updating option requires card input for the energy region to be altered. Data not supplied from cards are obtained from FISPROD.EVREG, FISPROD.KEVREG and FISPROD.MEVREG on FT units 10, 11 and 12 respectively. Any one or more of the 3 energy regions may be updated at a time, the data compilation being handled by the same procedure as in program FPLGP. The various additional options built into FPEDIT provide a fairly flexible means of updating the present fission product point cross section library. The point cross section library FISPROD.POINTXSL must be mounted on FT unit 13, and a temporary working file on FT unit 15.

3.3.2 Operating instructions

Input to FPEDIT

The fission product point cross section library if provided on tape must be loaded on tape unit 280, FT unit 13.

The input data deck consists of the following;

(i) card 1 contains

LIST, NU, NNUC, TITLE in format (I1,1XI2,1XI3,1X17A4)

where LIST is a counter for the options provided by the program and defined below,

NU = output FT unit number of the copied or updated library (either 9, 14, or $\geqslant$16); if LIST = 0 and NU = 0, listing option (on printer) only is used,

NNUC = number of nuclides to be handled,

TITLE = any required heading for the PRINTER output,

and LIST = 0 for listing and/or copying only

= 1 for updating only

= 2 for plotting of σ vs E graphs (on log-log scale) only

= 3 for combination of 0 and 2

= 4 for combination of 1 and 2

= 5 for combination of 2, 1, 2

(i.e. plotting of old data, then update, followed by plotting of new data)

(ii) for each nuclide to be edited, updated or plotted

card 1: NIC, IA = nuclide label in columns 1 to 5 (e.g. ZN672)

card 2: NX, RTN_i, (i = 1, NX) in format [I1,6(1XI4)]

where NX = number of reactions to be manipulated

RTN_i = reaction type number to be edited/updated/plotted in ascending order.

If NX = 6, RTN's need not be specified,

if NX = 4 or 5, the RTN's not required must be specified,

while for NX $\leqslant$ 3, the required RTN's are specified.

Sections (i) and (ii) only are required for an editing or plotting job. For LIST $\geqslant$ 3, section (ii) must be included for each option, since the RTN specification may be altered from option to option.

(iii) For update option only, following section (ii) for each nuclide.

Card 1 contains LOP, NXS in format [2(I1,1X)]

where LOP = 0 →7 with values;

0 for update of all regions using updated disk input files FISPROD.EVREG, FISPROD.KEVREG, FISPROD.MEVREG on FT units 10, 11, 12

1 for update of eV region data only

2 for update of keV region data only

3 for update of MeV region data only

4 for update of eV + keV regions

5 for update of eV + MeV

6 for update of keV + MeV

7 for update of all 3 regions (from cards)

NXS = number of cross section sets in card input.

Each updated region (LOP > 0) requires card input, while data for the non-updated region are available from the data files on disk pack 5.

Card input for eV region

Card 1: XSEC [format (2XA4)]

= either *(N,GAMMA) or *(N,TRANS)

followed by the appropriate cross section deck in format (6E12.5) as per GUNYA output.

If NXS = 2, data deck consists of

*(N,GAMMA)

127 $\sigma_{n\gamma}$ group values

*(N,TRANS)

127 $\sigma_{transport}$ group values

If NXS = 1, only one data set is given on cards, the other one being obtained from FISPROD.EVREG on FT unit 10.

Card input for keV region

Set of cards containing E, $\sigma_{n\gamma}$, σ_{total} per card in format (8XI3,32X2E10.2) as per FISPROD.KEVREG for 5 keV $\leqslant$ E $\leqslant$ 100 keV (same number of energy points as disk data file).

If NXS = 1, the non-required cross section is set to zero for all energy points, and is obtained from FISPROD.KEVREG on FT unit 11.

Card input for MeV region

Set of cards containing

Z, A, E, $\sigma_{n\gamma}$, $\sigma_{e\ell}$, $\sigma_{nn'}$, σ_{total} per card in format and energy grid of FISPROD.MEVREG. For NXS < 4, non-required cross sections are set to zero for all energies, and obtained from FISPROD.MEVREG on FT unit 12.

For LOP $\geqslant$ 4, the card input must be provided in order of eV, keV, MeV-card decks.

Output from FPEDIT

The layout and format of the copied and updated data sets are identical to those of FISPROD.POINTXSL. The output device NU for the copying and/or updating options is chosen by the user. All PRINTER output is self explanatory.

The plotting option, using the PDP-9 CALCOMP plotter, yields a graph for each required cross section as a function of energy on a log-log scale. Again PRINTER and plotting output are self-explanatory.

4. PROGRAMS BOMB, GPEDIT ASSOCIATED WITH FISPROD.GROUPXSL

4.1 The Group Averaging Program BOMB

4.1.1 Description

BOMB was written by G. Doherty (1969) to read cross section libraries in the layout and format of the U.K.A.E.A. Nuclear Data Library (Parker, 1963), and to compute group averaged cross section data for any required group structure. The program is on disk pack 5 with a catalogued procedure and reads the data from tape mounted on unit 280.

The averaging process is performed with the following assumptions;

(i) at high energy the flux is an integrated fission spectrum of the form

$$\phi(E) = \int_E^\infty f(E)\, dE$$

where $f(E) = a \sqrt{E}\, e^{-E/b}$,

with $a = 1.872$

$b = 1.290$

(ii) at intermediate energy the flux is constant in lethargy, i.e. $\phi(u)$ = constant

and $\phi(E) = \frac{1}{E}$

and (iii) at low energy the flux is Maxwellian of form

$$\phi(E) = \frac{E}{kT^2} \exp(-E/kT)$$

where T is temperature in degrees Absolute,

and k is Boltzmann's constant.

The changeover points for the various flux regions and the Maxwellian temperature T(°A) are specified by the user.

4.1.2 Input requirements

Card 1 = an eighty-column title card

Card 2 = option card in format (A4) containing either DUMP for listing of tape only or GROUP for group averaging only. If blank, both DUMP and GROUP options are used.

For group averaging, the following additional cards are required;

Card 3 = in free format, contains

NG = number of groups,

= 127 for a GYMEA library

Card 4 = in free format (columns 1 – 72) contains the (NG+1) group lethargy boundaries in ascending order,

normally: 0(.25)13.75,13.9(.1)20.5(.5)23.0

Card 5 = contains T, u_1, u_2, u_3, (in free format)

where T = Maxwellian Temperature in degrees Absolute; normally = 300 °A

u_1 = cutoff lethargy between high and intermediate energy flux regions, normally = 7.9

u_2 = cutoff lethargy between intermediate and low energy flux regions, normally = 18.9

and u_3 = lower cutoff of Maxwellian flux region, normally 50.0

Card 6 = contains NN = number of nuclides to be processed (free format),

Card 7 = contains the NN 'NIN' values of the nuclides to be processed (free format: columns 1 → 72).

The next NN cards (one per nuclide) contain, in free format, NJ = number of RTN's plus the NJ 'RTN' values.

The last card contains the variable LAST in free format where LAST takes the values 1 to 7, with

1 for printer output only
2 for punch output only
3 for printer and punch
4 for tape (or disk) on FT unit 12
5 for printer and tape (or disk)
6 for punch and tape (or disk)
7 for all 3 output devices.

4.2 The Editing and Updating Program GPEDIT

4.2.1 Description

The program GPEDIT, written to provide an editing, updating and plotting facility for the existing fission product group cross section library FISPROD.GROUPXSL handles the following options;

(i) listing and/or copying of any nuclide cross section set in the library,

(ii) updating of any cross section set from new data on cards, disk or tape,

(iii) plotting of log (σ) vs lethargy histograms for any cross section set, and special option

(iv) for preparing a correct and complete data file on disk or tape for input to the GYMEA cross section editing program XSEDIT.

A counter ℓ (0 → 5) is used to specify the first three options and combinations thereof, while $\ell = 6$ indicates option (iv) which cannot be run in conjunction with any of the other options. The updating option requires card (or disk/tape) input for the cross section sets to be replaced with the remaining cross sections either calculated from the appropriate formulae (Section 2.1.3) or obtained from the library FISPROD.GROUPXSL mounted on FT unit 14.

The subroutine FISGYM

Subroutine FISGYM must be specially mentioned and described here, because of its importance in the preparation of the data file FISPROD.GYMEAGP which is required as full input to the GYMEA cross section editing program XSEDIT for later generation of a GYMEA-type binary cross section library.

Since XSEDIT requires all input from a single device (ordinarily the card reader) the data file created by FISGYM must contain all the required XSEDIT control cards, burnup data, group and nuclide information as well as group cross section data for each nuclide. FISGYM provides the facility to merge card and tape input and produce a single input file on disk or tape. The input requirements of FISGYM and hence XSEDIT, are described later (Section 4.2.2).

This section deals with the special adaptations of the group cross section library FISPROD.GROUPXSL through subroutine FISGYM to meet the requirements of the GYMEA binary library structure.

Investigation of the fission product decay chains of England (1965) yields the fact that several nuclides decay by different (n,γ) reactions to two isomeric states. The GYMEA library handles this type of behaviour by introducing two reactions (1 and 6) for the parent nuclide in the ratio of ground state to isomeric state production, i.e. if r is the ratio of isomeric state to total production, then

$$\text{reaction (1)} = (1-r)\ \sigma_{n\gamma}$$

$$\text{reaction (6)} = r\ \sigma_{n\gamma} \quad .$$

The nuclides involved are ^{114}Cd, ^{122}Te, ^{124}Te, ^{126}Te, ^{128}Te, ^{130}Te and ^{147}Pm.

In addition ^{125}Sb β-decays by two modes to ^{125}Te and its isomer ^{125m}Te. However, as GYMEA allows for one β-decay specification only, this difficulty must be overcome in some way. Looking at the decay chain from ^{124}Sn onwards, it was found expedient to replace ^{125}Sn by two nuclides ^{125A}Sn and ^{125B}Sn, and ^{125}Sb by ^{125A}Sb and ^{125B}Sb, where the A series gives rise to ^{125}Te and B series yields the isomer ^{125m}Te. This method requires the splitting up of the (n,γ) reaction of ^{124}Sn into reactions (1) and (6) in the ratio of (1−r) /r.

A similar situation arises in the decay of ^{127}Sb to ^{127}Te and ^{127m}Te. Here the parent nuclide ^{127}Sb is replaced by 2 nuclides with ^{127A}Sb decaying to ^{127}Te and ^{127B}Sb to ^{127m}Te, and the ratio of reaction (1) of ^{127A}Sb to reaction (1) of ^{127B}Sb equals the ratio of ground to isomeric state production.

FISGYM was written to handle these cases automatically, expanding the 192 fission product group cross section library to one containing 195 nuclides. To perform this operation, FISGYM requires input of the ratios r_i and corresponding NIN's for all or some of the 9 nuclides involved.

Appendix 3 tabulates this ratio for each of the nine nuclides.

4.2.2 Operating instructions

Input to GPEDIT

Item (1) a card containing: LIST, NINP, NU, NNUC, TITLE in format [I1,2(1XI2),1XI3,1X17A4]

where LIST = the required option with values

0 for listing/copying only

1 for updating only

2 for plotting only

3 for combination of 0 + 2

4 for combination of 1 + 2

5 for combination of 2 + 1 + 2

and 6 for preparation of XSEDIT data file,

NINP = input device FT unit number for updating option, (if blank NINP = 1 i.e. card reader),

NU = output FT unit number for copying and updating options, also for FISGYM output file,

NNUC = number of nuclides to be treated,

and TITLE = 17 column heading for printer output.

Options LIST $\leq$ 5

Item (2) a card containing: NIC, IA in format (A2,I3)

where NIC = chemical symbol of nuclide

IA = atomic mass number,

Item (3) a card containing: NX, (RTN_i,i = 1,NX) in format [I1,6(1XI4)]

where NX = number of cross section blocks to be handled for above nuclide,

and RTN_i;i = 1, NX are the NX required reaction type numbers.

If NX = 6, no RTN's need be given,

if NX = 5 or 4, those not required are specified,

while for NX $\leq$ 3 those required are specified.

This completes the input requirements for the listing/copying and plotting options with items (2) and (3) repeated for each of the NNUC nuclides.

For the updating option the appropriate NX cross section sets must be provided on cards, disk or tape, for each nuclide, in ascending order of RTN and in the following layout and format:

Item (4) – a card/record containing the RTN in columns/bytes (11 → 14),

Item (5) – the 127 values, 6 per card/record, in format (6E12.5), of the particular reaction specified by the above RTN, followed by

Item (6) – a terminator card/record with *$$$$ . . . . . in columns/bytes 1 onwards.

Items (4) to (6) are repeated for each cross section, items (2) to (6) are repeated for each of the NNUC nuclides, each complete nuclide data set being terminated by a card/record containing *$*** : : : : : (columns/bytes 1 to 80).

For LIST ≥ 3, i.e. combinations of the three basic options, items (2) onwards must be supplied for each option, since the RTN specification and hence cross section data may be altered from option to option within a single run.

The output file on FT unit NU is in the same layout and format as the original group data library FISPROD.GROUPXSL which must be mounted on FT unit 14. All output on the printer is self explanatory.

Option LIST = 6

FISGYM may be run for any number of NNUC nuclides at a time starting from nuclide NP1, provided the preceding (NP1–1) nuclides are already in the library FISPROD.GYMEAGP, mounted on FT unit NU. A temporary working file must be available on FT unit 16 for NP1 >1 runs.

The following input is required by FISGYM to generate the XSEDIT input library FISPROD. GYMEAGP.

Card 1 as described above,

Card 2 contains: NP1, ISM, (ISOM (I), I = 1,ISM) in format [20(I3,1X)]

where NP1 = NIN of first nuclide to be treated

ISM = number of special nuclides

and ($ISOM_i$, i = 1,ISM) are the ISM NIN values for the special nuclides (see 4.2.1).

If ISM ≠ 0, card 3 must contain ISM values of the isomeric production ratio (RAT_i, i = 1,ISM) in format (6E12.5).

If ISM = 0, this card is omitted.

The next four input cards are control cards for XSEDIT and contain the following alphanumeric data in free format starting on column 1.

START IN,IOUT,IPERR

LAYOUT NLAY, (LAYOUT (I), I = 1,NLAY)

HEAD XS library name, short heading

PARAMETERS ID, NN, NG, IRS, IRT, PTEMP

where IN = 0 for initial library load

= FT unit number if binary library already exists

IOUT = required output unit for binary library generated by XSEDIT

IPERR = error indicator (=0)

NLAY = number of nuclides to be loaded

(= 187 for present library, 8 isomer to be added at a later date)

LAYOUT(I) = –1 for deletion of nuclide from existing binary library

= 0 for retrieval from binary library

= 1 for data supplied by cards, disk or tape

(LAYOUT(I) = 1 for initial load) .

If all nuclides are supplied in input the layout card becomes LAYOUT NLAY, NLAY * 1 .

ID = library update reference number for a first load (=1),

NN = number of nuclides supplied (187),

NG = number of groups in cross section data,

IRS,IRT = first and last resonance group,

and PTEMP = temperature of cross section data in degrees Absolute.

Then follow NN lots of data relating to burnup and nuclide information, each lot consisting of the following 3 cards:

DATA NUC, NAME, STATE, 0

BURNUP CH1, CH2, CH3, 0, DECAY, 4 * YIELDS

NUCLIDE 1.0, A, SGB, 7 * 0.

where NUC = nuclide identification [e.g. ZN72]

NAME = data set label [e.g. AAEC70]

STATE = ORIG for original data;

CH1, CH2, CH3 are the decay products for $\beta-$, $2(n\gamma)-$decays according to the fission product decay chains of England (1965),

DECAY = decay constant λ x 10^{24},

4 * YIELDS are the yields respectively from ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu,

A = atomic mass (floating point)

and SGB = σ_b, potential scattering cross section.

The next set of data is the group information consisting of the group lethargy boundaries, neutron fission spectrum values and group velocities. The group lethargy boundaries (u_i,i = 1,128) are obtained by FISGYM from the cross section input library FISPROD.GROUPXSL on FT unit 14. The following cards must be provided for the remaining data

FISSION SPECTRUM

(FSP_i,i = 1,127)

VELOCITIES

(v_i,i = 1,127)

plus a terminator *$\not{0}$*** . . . . . in columns 1 onwards.

The group cross section values for each reaction required by GYMEA are read from tape library FISPROD.GROUPXSL.

Comment cards may appear anywhere in the input deck (usually at end of "file") and will be stored as library comments if the first two columns contain ** .

This completes the card and tape (or disk) input requirements for subroutine FISGYM. For NP1 > 1 runs, the 4 control cards and the group information deck must be omitted. The group cross section library FISPROD.GROUPXSL must again be mounted on FT unit 14.

The XSEDIT input library FISPROD.GYMEAGP on disk or tape as specified, generated from the above input contains the following information in the correct layout and format. All records, again EBCDIC card images, are 80 bytes long and blocked to 7280.

'File' 1 consists of the 4 control statements

START . . . . .

LAYOUT . . . .

HEAD . . . . .

PARAMETERS . .

followed by the table of NN burnup and nuclide information sets:

DATA . . . . .

BURNUP. . . .

NUCLIDE . . .

followed by the group information:

GROUP

$(u_i, i = 1,128)$

FISSION SPECTRUM

$(FSP_i, i = 1,127)$

VELOCITIES

$(v_i, i = 1,127)$

*½*** . . . . . ***

'File' 2 contains the NN sets of cross section data in the order of the table generated in 'file' 1. Each nuclide block of cross section data consists of the following:

title record (as DATA above)

*(n,R1)

$127 * \sigma_{n\gamma}$ (=1102)

*(n,R2)

127 * 0.

*(n,R3)

$127 * \sigma_{abs}$ (=1102)

*(n,R4)

127 * 0.

*(n,R5)

$127 * \sigma_{trans}$ (=1201)

*(n,R6)

127 * 0. or next important reaction (see Section 4.2.1)

plus ** . . . . . any number of comment records.

The complete library is terminated by the control word END (bytes 1 to 3).

5. REFERENCES

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APPENDIX 1

FISSION PRODUCTS IN LIBRARY WITH ASSOCIATED NIN's

1	30ZN 72	49	42MO100	97	51SB128	145	60ND143
2	31GA 72	50	43TC 99	98	52TE122	146	60ND144
3	32GE 72	51	44RU100	99	52TE123	147	60ND145
4	32GE 73	52	44RU101	100	52TE124	148	60ND146
5	32GE 74	53	44RU102	101	52TE125	149	60ND147
6	32GE 76	54	44RU103	102	52TE126	150	60ND148
7	32GE 77	55	44RU104	103	52TE127	151	60ND150
8	33AS 75	56	44RU105	104	52TE128	152	61PM147
9	33AS 76	57	44RU106	105	52TE129	153	61PM148
10	33AS 77	58	45RH103	106	52TE130	154	61PM149
11	34SE 76	59	45RH105	107	52TE131	155	61PM151
12	34SE 77	60	46PD104	108	52TE132	156	62SM147
13	34SE 78	61	46PD105	109	53I 127	157	62SM148
14	34SE 79	62	46PD106	110	53I 129	158	62SM149
15	34SE 80	63	46PD107	111	53I 130	159	62SM150
16	35BR 81	64	46PD108	112	53I 131	160	62SM151
17	35BR 82	65	46PD109	113	53I 133	161	62SM152
18	36KR 82	66	46PD110	114	53I 135	162	62SM153
19	36KR 83	67	46PD112	115	54XE128	163	62SM154
20	36KR 84	68	47AG109	116	54XE130	164	62SM156
21	36KR 85	69	47AG111	117	54XE131	165	63EU153
22	36KR 86	70	48CD110	118	54XE132	166	63EU154
23	37RB 85	71	48CD111	119	54XE133	167	63EU155
24	37RB 86	72	48CD112	120	54XE134	168	63EU156
25	37RB 87	73	48CD113	121	54XE135	169	63EU157
26	38SR 86	74	48CD114	122	54XE136	170	64GD155
27	38SR 88	75	48CD115	123	55CS133	171	64GD156
28	38SR 89	76	48CD116	124	55CS134	172	64GD157
29	38SR 90	77	49IN115	125	55CS135	173	64GD158
30	38SR 91	78	50SN115	126	55CS136	174	64GD159
31	39Y 89	79	50SN116	127	55CS137	175	64GD160
32	39Y 90	80	50SN117	128	56BA134	176	65TB159
33	39Y 91	81	50SN118	129	56BA136	177	65TB160
34	39Y 93	82	50SN119	130	56BA137	178	65TB161
35	40ZR 90	83	50SN120	131	56BA138	179	66DY160
36	40ZR 91	84	50SN121	132	56BA140	180	66DY161
37	40ZR 92	85	50SN122	133	57LA139	181	66DY162
38	40ZR 93	86	50SN123	134	57LA140	182	66DY163
39	40ZR 94	87	50SN124	135	58CE140	183	66DY164
40	40ZR 95	88	50SN125	136	58CE141	184	67HO165
41	40ZR 96	89	50SN126	137	58CE142	185	43TC799
42	40ZR 97	90	51SB121	138	58CE143	186	48CD815
43	41NB 95	91	51SB122	139	58CE144	187	52TE823
44	42MO 95	92	51SB123	140	59PR141	188	52TE825
45	42MO 96	93	51SB124	141	59PR142	189	52TE827
46	42MO 97	94	51SB125	142	59PR143	190	52TE829
47	42MO 98	95	51SB126	143	59PR145	191	52TE831
48	42MO 99	96	51SB127	144	60ND142	192	61PM848

APPENDIX 2

FISSION PRODUCTS WITH LAST RESOLVED RESONANCE ENERGY > 5 keV

Nuclide	Last Resolved Resonance Energy E_R (MeV)	Cut-off Group Energy Boundary E_ℓ for eV Region Data (MeV)
^{76}Se	5.160×10^{-3}	5.531×10^{-3}
^{85}Rb	5.8×10^{-3}	7.102×10^{-3}
^{86}Sr	1.16×10^{-2}	1.171×10^{-2}
^{90}Zr	1.73×10^{-2}	1.931×10^{-2}
^{91}Zr	5.6×10^{-3}	7.102×10^{-3}
^{92}Zr	4.7×10^{-2}	5.531×10^{-3}
^{94}Zr	1.975×10^{-2}	2.479×10^{-2}
^{96}Zr	5.97×10^{-3}	7.102×10^{-3}
^{141}Pr	5.732×10^{-3}	7.102×10^{-3}

APPENDIX 3

NINE SPECIAL NUCLIDES IN DECAY CHAINS

Parent Nuclide		Decay Products		Ratio of Isomeric State to Total Production
Chemical Symbol	NIN	Ground State	Isomer	
^{114}Cd	74	^{115}Cd	^{115m}Cd	0.1200
* ^{124}Sn	87	^{125A}Sn ^{125A}Sb ^{125}Te	^{125B}Sn ^{125B}Sb ^{125m}Te	0.2992
^{122}Te	98	^{123}Te	^{123m}Te	0.1000
^{124}Te	100	^{125}Te	^{125m}Te	0.1000
^{126}Te	102	^{127}Te	^{127m}Te	0.1000
^{128}Te	104	^{129}Te	^{129m}Te	0.0800
^{130}Te	106	^{131}Te	^{131m}Te	0.0500
^{147}Pm	152	^{148}Pm	^{148m}Pm	0.4724

* 2 β–decays