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RGENDF - AN INTERFACE PROGRAM BETWEEN THE NJOY CODE AND CODES USING MULTIGROUP CROSS-SECTIONS

E.S. Chalhoub, Jaime Anaf

Technical Note - IEAv-013/87 (September 1987)
Ministry of Aeronautics
Department of Research and Development
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Translated by the IAEA

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ABSTRACT

An interface program for reformatting multigroup cross-section libraries generated by NJOY into ENDF/B-V format and the EXPANDA, PFCOND and COMPAR input formats is presented.

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CONTENTS

1. INTRODUCTION

This report describes the "RGENDF" program, the purpose of which is to read the "GENDF" library produced by the "GROUPR" module of the NJOY code [1] and to create a new library suitable for other codes.

The "RGENDF" program is based on an earlier version, the purpose of which was to generate a library for the EXPANDA code [2]. It is capable of interpreting only the neutron data generated by NJOY, and does not accept the structure of gamma groups.

In the following sections, information will be presented on: formatting of the "GENDF" library, reactions that can be processed, storage of data by the program and formatting of the libraries produced. Appendix A includes: a description of the input and output files, a description of the input data, examples of input data for the libraries to be generated, data relating to dimensioning limitations and the control cards necessary for execution.

2. INPUT LIBRARY - "GENDF"

The "GENDF" library, produced by NJOY, can contain multigroup data for various materials. Each material (m) can present information for more than one temperature (t), and each temperature is divided into a number of files. The files (MF) 1, 3, 5 and 6 - the only ones read by RGENDF - contain the following information:

MF=1 the values of σ_0 (reference cross-section - "Background") in barns and the energy group structure in eV;

MF=3 the neutron cross-sections;

MF=5 the energy distributions of secondary neutrons; and

MF=6 the angular and energy distributions of secondary neutrons (transfer matrices).

Files 3, 5 and 6 are divided into various sections, each of which represents a nuclear reaction (in barns) for each energy group (g), in ascending order, for each value of $\sigma_0(s_0)$ and for each order of Legendre polynomial (ℓ-1).

The "GENDF" must be in the "BCD" format and must contain, apart from files 3 and/or 6, file 1, which is used in verifying the values of σ_0 employed in the processing.

3. NUCLEAR REACTIONS PROCESSED BY RGENDF

The names (Vector) assigned to the reactions (MT) processed by this program are shown in Table 1. Of the reactions specified, the only ones that are not read from the "GENDF", but calculated by the program, are:

(a) Elastic removal cross-section;

(b) Absorption cross-section (MF=3, MT=100); and

(c) Inelastic scattering matrix (MF=6, MT=4).

The elastic removal cross-section, for each energy group, is calculated on the basis of the sum of the elastic cross-sections of the neutrons migrating from each group towards the others, that is:

$$\sigma^{g}_{re} = \sum_{g' \neq g}^{G} \sigma_{e.g \to g'} \quad .$$

The absorption cross-section is calculated by means of the expression:

$$\sigma^{g}_{a} = \sigma^{g}_{tot} - \sigma^{g}_{e} - \left(\sigma^{g}_{in} + 2\,\sigma^{g}_{(n,2n)} + 3\,\sigma^{g}_{(n,3n)} \right) \quad ,$$

it being necessary to request at least the reactions σ^{g}_{tot} and σ^{g}_{e}.

The inelastic scattering matrix is determined by the sum of the matrices of the excited states (reactions 51 to 90) and of the continuum (reaction 91) from file 6.

4. DATE STORAGE

The data for the reactions in files 3, 5 and 6 are stored by the program in Vectors, in the following form: for

<u>R3001</u>
$((((R(g,s_0,\ell,t,m);\ g=1,G),\ s_0=1,S_0),\ell=1,L),\ t=1,T),\ m=1,M);$

<u>R3002, R0002, R3018, R3100 e R3102</u>
$(((R(g,s_0,t,m);\ g=1,G),\ s_0=1,S_0),\ t=1,T),\ m=1,M);$

<u>R3004, R3016, R3017 e R3103 a R3452</u>
$((R(g,t,m);\ g=1,G),\ t=1,T),\ m=1,M);$

<u>R5018</u>
$((R(g,m);\ g=1,G),\ m=1,M);$

<u>R6002</u>
$((((((R(g \to g',s_0,\ell,t,m);\ g=1,G),\ g'=1,G),\ s_0=1,S_0),\ \ell=1,L),$
$t=1,T),\ m=1,M);$

<u>R6004</u>
$((((((R(g \to g',\ell,t,m);\ g=1,G),\ g'=1,G),\ \ell=1,L),\ t=1,T),\ m=1,M);$

<u>R6016 e R6017</u>
$(((((R(g \to g',t,m);\ g=1,G),\ g'=1,G),\ t=1,T),\ m=1,M);$

where L is the maximum order of the Legendre polynomial + 1, and G, S_0, T and M are the total numbers of: energy groups, reference cross-sections, temperatures and materials.

In storing the data, a set of sub-routines developed specifically for the dynamic allocation of variables is used [3].

5. LIBRARIES PRODUCED

The RGENDF program creates libraries depending on a control variable provided as an item of input data. Each library is produced by a specific sub-routine which carries out calculations as required, together with the necessary formatting.

The RGENDF is a structured program. The insertion of new formatting sub-routines, in accordance with the block diagram shown in Fig. 1, involves slight alterations in the main program and in the RFIND sub-routine. The variables JCODE and NMAT, shown in the diagram, are described in Appendix A.

In its present version, the RGENDF can produce four different libraries through the sub-routines WEXPAND, WPFCOND, WCOMPAR and WENDFBV, which generate data for the EXPANDA [3], PFCOND [4] and COMPAR [5] codes and in the ENDF/B-V [6] format, respectively. We shall now describe the structures of these libraries.

5.1. Structure of the WEXPAND library

This library is generated in binary format, with two types of register. The first register contains control parameters and data necessary for interpreting the second register and for processing the EXPANDA code:

MCODE(m), m=1,M

Identification of the materials, in accordance with JAERI [6].

MSF(m), m=1,M

Control variable indicating, for each material, values of σ_0 used in composing the tables of self-shielding factors, to be supplied in the second data register. For

MSF=1, σ_0 = 0,10,100,1000,10 000,100 000;
MSF=2, σ_0 = 0,1,10,100,1000,10 000; and
MSF=0, no value. In this way the data contained in the tables of self-shielding factors are set equal to unity.

CHI(g); g=1,G

Normalized fission spectrum.

TEMP(t); t=1,3

Temperatures in degrees K (300, 900 and 2100 K).

TAB1(i); i=1,6

Constants for interpolation (used when MFS=1).

TAB2(i); i=1,6

Constants for interpolation (used when MFS=2).

AM(m); m=1,M

Atomic masses of the materials.

DU(g); g=1,G

Lethargy width of the groups.

The second data register, divided into two parts, contains the multigroup constants and is repeated for each energy group, starting with the highest-energy group. The first part refers to the constants obtained for infinite dilution ($\sigma_0 = \infty$) and to a temperature of 300 K:

$$\sigma_f, \bar{\nu}_f, \sigma_c, \sigma_{in}, \sigma_e, \bar{\mu}, \sigma_{re},$$
$$\sigma_e(g \rightarrow g'); \; g' = 1,30,$$
$$\sigma_{in}(g \rightarrow g'); \; g' = 1,30,$$

each of these reactions being supplied as:

$\sigma_x(m)$; m = 1,M.

The second part refers to the self-shielding factors obtained for six values of σ_0 (in accordance with the variable MSF) and to three temperatures (300, 900 and 2100 K).

$$F_{f_1}, F_{f_2}, F_{c_1}, F_{c_2}, F_{e_1}, F_{e_2}, F_{tot_1}, F_{tot_2}, F_{re_1} \text{ e } F_{re_2}$$

represent the cross-section for the fission, capture, elastic, total and elastic removal reactions, respectively, calculated for two atomic density ratios of two resonant nuclei [6]. Each of these factors is supplied in the following manner:

$F_x(s_0,t,m)$; $s_0 = 1,6$, $t = 1,3$, $m = 1,M$.

In case of non-existence of one of these reactions, the corresponding data contained in the tables of F_x factors are set equal to unity.

5.2. Structure of the WPFCOND library

The library is generated in the BCD format, and has the following three sets of registers:

1st set: constants (format 2I5)

a - M,G
Number of materials and number of energy groups;

b - MAT, NRP
Identification of the material according to ENDF/B and the number of reactions processed for this material;

2nd set: the number of the reaction and the corresponding multigroup cross-sections, starting with the lowest-energy group (format 1X, A4,/, (1P10E13.6))

c - IR,(σ_{tot} (g); g = 1,G) (IR = 3001)
Total reaction;

d - IR,(σ_e (g); g = 1,G) (IR = 3002)
Elastic reaction;

e - IR,(σ_{in} (g); g = 1,G) (IR = 3004)
Inelastic reaction;

f - IR,($\sigma_{(n,2n)}$ (g); g = 1,G) (IR = 3016)
(n,2n) reaction;

g - IR,($\sigma_{(n,3n)}$ (g); g = 1,G) (IR = 3017)
(n,3n) reaction;

h - IR,($\bar{\mu}$(g); g = 1,G) (IR = 3251)
Mean cosine of the scattering angle;

<u>3rd set</u>: the number of the reaction and the corresponding transfer matrices (format 1X,A4,/, (1P10E13.6))

i - IR,((σ_e (g → g'); g' = 1,G), g = 1,G) (IR = 6002)
Elastic matrix;

j - IR,((σ_{in} (g → g'); g' = 1,G), g = 1,G) (IR = 6004)
Inelastic matrix;

k - IR,(($\sigma_{(n,2n)}$ (g → g'); g' = 1,G), g = 1,G) (IR = 6016)
(n,2n) matrix;

ℓ - IR,(($\sigma_{(n,3n)}$ (g → g'); g' = 1,G), g = 1,G) (IR = 6017)
(n,3n) matrix.

The registers b to ℓ are repeated M times.

5.3. Structure of the WENDFBV library

This library is generated in the ENDF/B-V format, and contains only files 1 and 3. In order to give a better picture, part of it is shown in Table 2, and its structure is given as:

<u>File 1</u>:

[MAT,1,451/ZA,AWR,0,LFI,0,0] HEAD
[MAT,1,451/0.,0.,0,0,0,0] CONT
[MAT,1,451/SIGO,0.,0,0,NWD,NXC/ZSYMA/H(N)] LIST
[MAT,1,451/0.,0.,MF_1,MT_1,NC_1,0] CONT
[MAT,1,451/0.,0.,MF_2,MT_2,NC_2,0] CONT
.
.
.
[MAT,1,451/0.,0.,MF_{NXC},MT_{NXC},NC_{NXC},0] CONT
[MAT,1, 0/0.,0.,0,0,0,0] SEND
[MAT,0, 0/0.,0.,0,0,0,0] FEND

<u>File 3</u>:

[MAT,3, MT/ZA,AWR,0,0,LORD,IS] HEAD
[MAT,3, MT/S,0.,0,0,1,NGR2/E_{int}/$\bar{\sigma}$] TAB1
[MAT,3, 0/0.,0.,0,0,0,0] SEND

These cards are repeated for each reaction processed, the library concluding with the following cards:

```
[MAT,0,  0/0.,0.,0,0,0,0]   FEND
[  0,0,  0/0.,0.,0,0,0,0]   MEND
[ -1,0,  0/0.,0.,0,0,0,0]   TEND
```

where:

- MAT is the number of the material according to ENDF/B;
- ZA is equal to (1000.*Z)+A, where Z is the atomic number and A the mass number of the material;
- AWR is the ratio between the masses of the material and that of the neutron;
- LFI indicates whether the material is fissile (=1) or not (=0);
- SIGO is the σ_0 used in processing;
- NWD is the number of cards which describe the material;
- NXC is the number of sections contained in the dictionary;
- ZSYMA is the symbolic representation of the material, in columns 1 to 11;
- H(N) is the title containing information which describes the manner in which the material was processed;
- MF_i is the file of the i-th section;
- MT_i is the reaction of the i-th section;
- NC_i is the number of cards contained in the i-th section;
- MT is the reaction processed;
- LORD is the Legendre order;
- IS is the i-th value of σ_0 used in processing;
- S is the temperature in degrees K;
- NGR2 is given as 2*(G+1), G being the number of energy groups;
- E_{int} is the interpolation scheme used; and
- $\bar{\sigma}$ are the multigroup cross-sections given as: $E_1\ \sigma_1\ E_2\ \sigma_2 \ldots E_g\ \sigma_g\ E_{g+1}\ \sigma_{g+1} \ldots E_G$ $\sigma_G\ E_{G+1}\ 0$, σ_g being valid in the group bounded by the energies E_g and E_{g+1}.

5.4. Structure of the WCOMPAR library

The library is generated in the BCD format with two data registers:

1st register (format 3I5)

MAT,NGR,NUTHG
Number of the material according to ENDF/B, number of energy groups and number of the highest-energy thermal group;

2nd register (format I5, 1P3E15.5)

$g, \sigma_e^g, \sigma_f^g, \sigma_c^g;$ $g = 1,G.$

These two registers are repeated for each material, the library ending with MAT = -1. In the case of the first register alone, a title, in the "6A10" format, is provided together with the variables MAT, NGR and NUTHG, resulting in (3I5,6A10).

6. REFERENCES

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[4] ONO, Shizuca, PAVIOTTI CORCUERA, R., "Preparation of the cross-sections of condensed fission products for a multigroup library" [in Portuguese], Technical Note - IEAv/NT-013/84, 1984.

[5] ANAF, Jaime, CHALHOUB, E.S., "COMPAR - A system for comparing multigroup cross-sections generated by NJOY, GROUPIE, FLANGEII, ETOG3 and XLACS" [in Portuguese], IEAV-014/87 (November 1987).

[6] "Data formats and procedures for the evaluated nuclear data file, ENDF/B-V", Brookhaven National Laboratory, BNL-NCS-50496 (ENDF-102), (1983).

[7] TANAKO, H., HASEGAWA, A., NAKAGAWA, M., ISHIGURO, Y., KATSURAGI, S., "JAERI fast reactor group constants set, Version II", JAERI-1255 (1978).

Table 1: Reactions processed by RGENDF

MF	MT	VECTOR	REACTION
3	1	R3001	Total (tot)
	2	R3002	Elastic (e)
	-	R0002	Elastic removal (re)
	4	R3004	Inelastic (in)
	16	R3016	(n,2n)
	17	R3017	(n,3n)
	18	R3018	Fission (f)
	100	R3100	Absorption (a)
	102	R3102	(n,γ) - Capture (c)
	103	R3103	(n,p)
	104	R3104	(n,d)
	105	R3105	(n,t)
	106	R3106	(n,^{3}He)
	107	R3107	(n,α)
	251	R3251	$\bar{\mu}$ - mean cosine of the scattering angle
	252	R3252	ξ - mean logarithmic energy decrement for elastic scattering
	253	R3253	γ - mean square decrement of the energy logarithm divided by 2ξ.
	259	R3259	1/v - reciprocal of the velocity
	452	R3452	$\bar{\nu}$ - average number of neutrons released through fission
5	18	R5018	Normalized fission spectrum
6	2	R6002	Elastic matrix (e)
	4	R6004	Inelastic matrix (in)
	16	R6016	(n,2n) matrix
	17	R6017	(n,3n) matrix

Table 2: Library in the ENDF/B-V format

```
                                                                          0 0  0     0
2.70590+04 5.84269+01          0          0          0          06327 1451     1
0.00000+00 0.00000+00          0          0          0          06327 1451     2
1.00000+10 0.00000+00          0          0         10          46327 1451     3
27-CO-59                                                         C6327 1451     4
THIS MATERIAL HAS BEEN PROCESSED, AT CTA/IEAV, IN A COMPUTER     H6327 1451     5
COC 170/750, JUL/82, BY HJOY (10/81-2), WITH A FRACTIONAL        A6327 1451     6
RECONSTRUCTION TOLERANCE OF 0.005, UTILIZING THE ENOF/B-V,       L6327 1451     7
MOD 1, OOSIMETRY LIBRARY, TO PREPARE 620 GROUP (SAHO-II          H6327 1451     8
STRUCTURE) GROUP AVERAGES FOR UNSHIELDEO, COLO (0 KELVIN)        D6327 1451     9
AND FLAT WEIGHTED.                                               U6327 1451    10
ALL CROSS SECTIONS ARE GIVEN IN FILE 3.                          B6327 1451    11
                                                                  6327 1451    12
                                                                  6327 1451    13
                               1        451         17          06327 1451    14
                               3         16        210          06327 1451    15
                               3        102        210          06327 1451    16
                               3        107        210          06327 1451    17
                                                                  6327 1  0    18
                                                                  6327 0  0    19
2.70590+04 5.84269+01          0          0          0          06327 3 16    20
0.00000+00 0.00000+00          0          0          1       12426327 3 16    21
      1242          2                                            6327 3 16    22
1.00000-04 0.00000+00 1.05000-04 0.00000+00 1.10000-04 0.00000+006327 3 16    23
1.15000-04 0.00000+00 1.20000-04 0.00000+00 1.27500-04 0.00000+006327 3 16    24

  (MISSING LINES)

1.75000+07 8.64500-01 1.76000+07 8.63500-01 1.77000+07 8.62500-016327 3 16   228
1.78000+07 8.61500-01 1.79000+07 8.60500-01 1.80000+07 0.00000+006327 3 16   229
                                                                  6327 3  0   230
2.70590+04 5.84269+01          0          0          0          06327 3102   231
0.00000+00 0.00000+00          0          0          1       12426327 3102   232
      1242          2                                            6327 3102   233
1.00000-04 5.85609+02 1.05000-04 5.71428+02 1.10000-04 5.59364+026327 3102   234
1.15000-04 5.48189+02 1.20000-04 5.34221+02 1.27500-04 5.17542+026327 3102   235

  (MISSING LINES)

1.75000+07 5.94000-04 1.76000+07 5.82000-04 1.77000+07 5.70000-046327 3102   439
1.78000+07 5.58000-04 1.79000+07 5.46000-04 1.80000+07 0.00000+006327 3102   440
                                                                  6327 3  0   441
2.70590+04 5.84269+01          0          0          0          06327 3107   442
0.00000+00 0.00000+00          0          0          1       12426327 3107   443
      1242          2                                            6327 3107   444
1.00000-04 0.00000+00 1.05000-04 0.00000+00 1.10000-04 0.00000+006327 3107   445
1.15000-04 0.00000+00 1.20000-04 0.00000+00 1.27500-04 0.00000+006327 3107   446

  (MISSING LINES)

1.75000+07 1.85800-02 1.76000+07 1.81400-02 1.77000+07 1.77133-026327 3107   650
1.78000+07 1.73667-02 1.79000+07 1.70333-02 1.80000+07 0.00000+006327 3107   651
                                                                  6327 3  0   652
                                                                  6327 0  0   653
                                                                     0 0  0   654
                                                                    -1 0  0     0
```

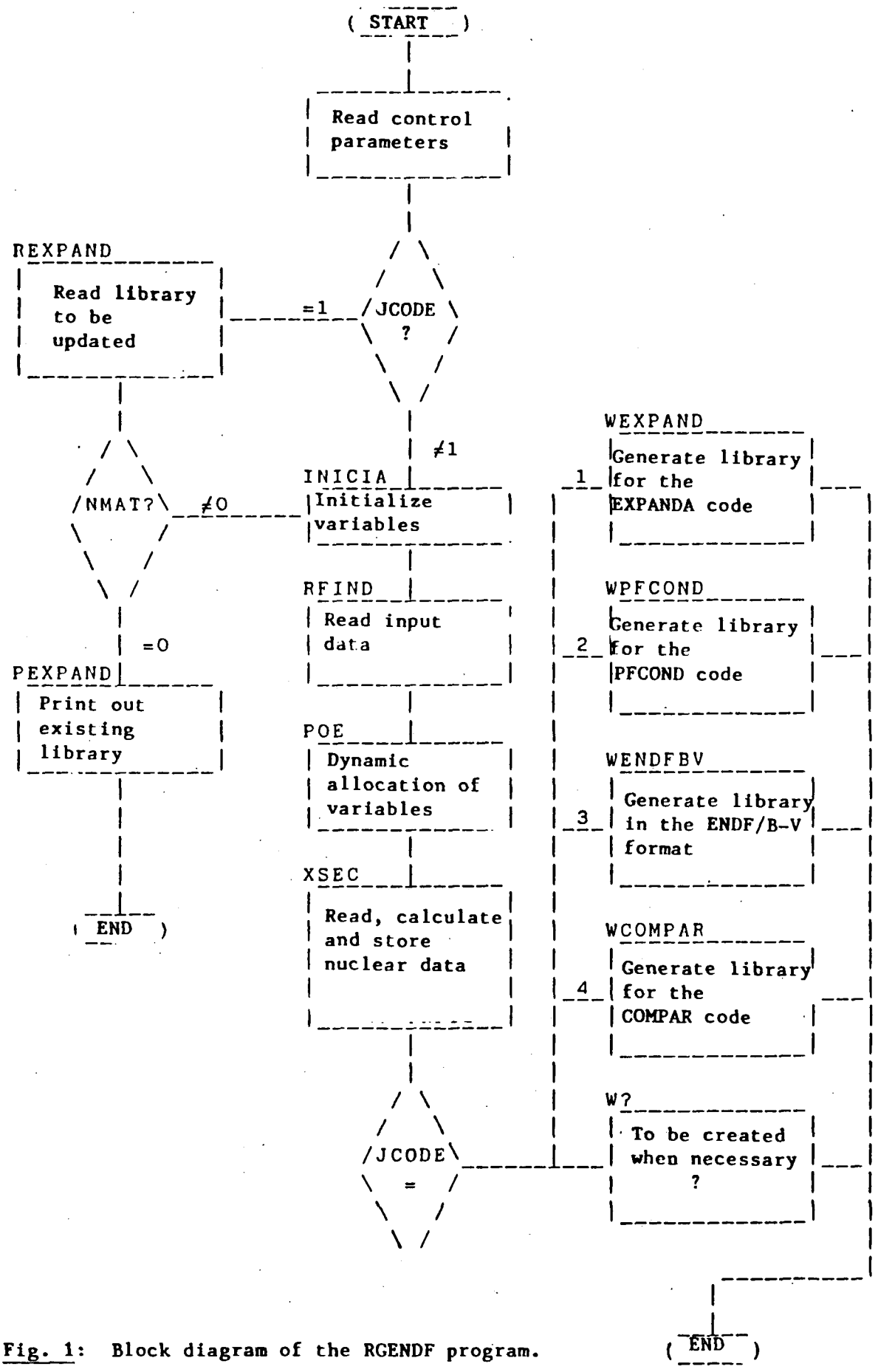

Fig. 1: Block diagram of the RGENDF program.

APPENDIX A

[Translation of lines RGEN0006 to RGEN0322:]

Purpose

The purpose of this programme is to read the ≠GENDF≠ library produced by the ≠GROUPR≠ module of the ≠NJOY≠ code and to produce a new library that is suitable for other codes.

This program was developed by Ezzat Selim Chalhoub and Jaime Anaf.
(Cards 14 to 151 omitted, since the the subject is covered in sections 2-4).

Input and output files

Input

1	Library produced by NJOY, containing the materials to be processed.
5	Input data.
7	Existing library to be updated, only if JCODE = 1.

Output

6	Printout.
8	New library, created or updated (if JCODE = 1).

Input data

Card 1 (Format 16I5)

JCODE Control variable indicating the desired format of the library to be produced.

JCODE = 1, library to be processed by the EXPANDA-70D code.
JCODE = 2, library to be processed by the PFCOND code.
JCODE = 3, library in the ENDF/B-V format.
JCODE = 4, library to be processed by the COMPAR code.

NMAT Number of materials to be processed. Maximum five materials per processing permitted, owing to the limitations imposed by the memory of the CDC-CYBER 170/750. This restriction is applied only for JCODE = 1. For the remaining options of JCODE, there is no restriction, since the program processes each material separately. See limitations mentioned below.

NMAT > 0, NMAT materials will form a new library. They will be added to an existing library, when JCODE = 1.

NMAT < 0, (only for JCODE = 1)
ABS (NMAT) materials will be replaced in an existing library.

NMAT = 0, (only for JCODE = 1)
A list of the materials contained in an existing library will be printed. In this case, it is necessary to supply only the NWD variable of this card and the type-2 card.

APÊNDICE A

```
      PROGRAM RGENDF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE1,        RGEN0001
     1                TAPE2,TAPE3,TAPE4,TAPE7,TAPE8,TAPE9)               RGEN0002
C                                                                        RGEN0003
C     ***********************************************************        RGEN0004
C                                                                        RGEN0005
C     FINALIDADE                                                         RGEN0006
C     **********                                                         RGEN0007
C                                                                        RGEN0008
C     ESTE PROGRAMA TEM POR FINALIDADE LER A BIBLIOTECA #GENDF# PRODU-   RGEN0009
C     ZIDA PELO MODULO #GROUPR#, DO CODIGO #NJOY#, E PRODUZIR UMA NOVA   RGEN0010
C     BIBLIOTECA ADEQUADA A OUTROS CODIGOS.                              RGEN0011
C     ESTE PROGRAMA FOI ELABORADO  POR  EZZAT SELIM CHALHOUB  E  JAIME   RGEN0012
C     ANAF.                                                              RGEN0013


(CARTOES DE 14 A 151 RETIRADOS POR ESTAR O ASSUNTO INCLUIDO NOS CAPITULOS 2 A 4)


C     ARQUIVOS DE ENTRADA E SAIDA                                        RGEN0152
C     ***************************                                        RGEN0153
C                                                                        RGEN0154
C       ENTRADA                                                          RGEN0155
C       *******                                                          RGEN0156
C                                                                        RGEN0157
C         1       BIBLIOTECA PRODUZIDA POR  NJOY, CONTENDO OS MATERIAIS  RGEN0158
C                 A SEREM PROCESSADOS.                                   RGEN0159
C         5       DADOS DE ENTRADA.                                      RGEN0160
C         7       BIBLIOTECA  JA  EXISTENTE  A SER  ATUALIZADA, SOMENTE  RGEN0161
C                 SE JCODE=1.                                            RGEN0162
C                                                                        RGEN0163
C       SAIDA                                                            RGEN0164
C       *****                                                            RGEN0165
C                                                                        RGEN0166
C         6       IMPRESSAO DE SAIDA.                                    RGEN0167
C         8       BIBLIOTECA NOVA, CRIADA OU ATUALIZADA (SE JCODE=1).    RGEN0168
C                                                                        RGEN0169
C                                                                        RGEN0170
C                                                                        RGEN0171
C     DADOS DE ENTRADA                                                   RGEN0172
C     ****************                                                   RGEN0173
C                                                                        RGEN0174
C       CARTAO  1           FORMATO(16I5)                                RGEN0175
C         JCODE             VARIAVEL DE CONTROLE  INDICANDO  O  FORMATO  RGEN0176
C                           DESEJADO DA BIBLIOTECA A SER PRODUZIDA.      RGEN0177
C                             JCODE = 1, BIBLIOTECA  A  SER  PROCESSADA  RGEN0178
C                                        PELO CODIGO EXPANDA-70D.        RGEN0179
C                             JCODE = 2, BIBLIOTECA  A  SER  PROCESSADA  RGEN0180
C                                        PELO CODIGO PFCOND.             RGEN0181
C                             JCODE = 3, BIBLIOTECA    NO   FORMATO  DA  RGEN0182
C                                        ENDF/B-V.                       RGEN0183
C                             JCODE = 4, BIBLIOTECA  A  SER  PROCESSADA  RGEN0184
C                                        PELO CODIGO COMPAR.             RGEN0185
C         NMAT              NUMERO DE MATERIAIS A SEREM PROCESSADOS. NO RGEN0186
C                           MAXIMO 5 MATERIAIS, POR  PROCESSAMENTO, SAO RGEN0187
C                           PERMITIDOS, DEVIDO A LIMITACAO IMPOSTA PELA RGEN0188
C                           MEMORIA DO CDC-CYBER 170/750.  ESTA RESTRI- RGEN0189
C                           CAO EH APLICADA SOMENTE PARA  JCODE=1 .     RGEN0190
C                           PARA AS DEMAIS OPCOES DE JCODE, NAO HA RES- RGEN0191
C                           TRICAO, POIS O PROGRAMA PROCESSA  CADA  MA- RGEN0192
C                           TERIAL ISOLADAMENTE.VER LIMITACOES APRESEN- RGEN0193
C                           TADAS ABAIXO.                               RGEN0194
C                             NMAT > 0, NMAT MATERIAIS   FORMARAO   UMA RGEN0195
C                                       NOVA BIBLIOTECA.  SERAO ADICIO- RGEN0196
C                                       NADOS A UMA BIBLIOTECA JA EXIS- RGEN0197
C                                       TENTE, CASO JCODE=1 .           RGEN0198
C                             NMAT < 0, (SOMENTE PARA JCODE=1)          RGEN0199
C                                       ABS(NMAT) MATERIAIS SERAO SUBS- RGEN0200
C                                       TITUIDOS  NUMA   BIBLIOTECA  JA RGEN0201
C                                       EXISTENTE.                      RGEN0202
C                             NMAT = 0, (SOMENTE PARA JCODE=1)          RGEN0203
C                                       UMA RELACAO DOS MATERIAIS  CON- RGEN0204
C                                       TIDOS NUMA BIBLIOTECA  JA EXIS- RGEN0205
```

NGR	Number of energy groups. The data will be produced in order NGR < 0, decreasing in energy. NGR > 0, increasing in energy. The maximum values permitted are: NGR = 70, for JCODE = 1 and 2, and NGR = 620, for the remaining options.
NFIS	(omitted for JCODE = 2) Number of materials containing the fission cross-section (MAX NFIS = NMAT) to be processed.
NSIGO	(omitted for JCODE = 2) Number of reference cross-sections ≠BACKGROUND≠ (SIGMA-ZERO). The maximum values permitted are: NSIGO = 7, for JCODE = 1, and NSIGO = 8, for the remaining options.
NT	(omitted for JCODE < 3) Number of temperatures (max 6).
NPN	(omitted for JCODE < 3) Legendre order + 1 - (max 5).
NWD	(omitted for JCODE = 2) Number of comment cards to be supplied in the type-2 card. NWD(max) = 9, only for JCODE = 3 NWD = 1, for the remaining options.
NUTHG	(necessary if JCODE = 4) Number of the highest-energy thermal group.
IPRINT	Control variable for the printing (= 1) or not (= 0) of a table containing the dimensioning of the variables, effected by dynamic allocation.
Card 2 ((TIT(I,J), I = 1, 6), J = 1, NWD)	Format (6A10) - (omitted for NWD = 0) Title to be given to the library produced.
Card 3 (T(IT), IT = 1,NT)	Format (8E10.5) - (omitted for JCODE < 3) Temperature in degrees K.
Card 4 (SIGO(IS), IS = 1, NSIGO)	Format (8E10.5) - (omitted for JCODE < 3) Values of reference cross-sections ≠BACKGROUND≠ (SIGMA-ZERO) in barns.
Card 5 (MATD(IM), IM = 1, ABS(NMAT)	Format (5I5) - (omitted for NMAT = or > 0). Identification of the materials, according to JAERI, to be substituted in an existing library.

```
C                                        TENTE, SERA IMPRESSA.  NESTE  RGEN0206
C                                        CASO, EM NECESSARIO FORNECER  RGEN0207
C                                        APENAS A VARIAVEL NWD DESTE  RGEN0208
C                                        CARTAO E O CARTAO DO TIPO 2.  RGEN0209
C          NGR                 NUMERO DE GRUPOS DE ENERGIA.                RGEN0210
C                              OS DADOS SERAO PRODUZIDOS EM ORDEM          RGEN0211
C                                NGR < 0, DECRESCENTE DE ENERGIA.          RGEN0212
C                                NGR > 0, CRESCENTE DE ENERGIA.            RGEN0213
C                              OS VALORES MAXIMOS PERMITIDOS SAO:          RGEN0214
C                                NGR =  70, PARA JCODE=1 E 2   E           RGEN0215
C                                NGR = 620, PARA AS DEMAIS OPCOES.         RGEN0216
C          NFIS                (OMITIDO PARA JCODE=2)                      RGEN0217
C                              NUMERO DE MATERIAIS A SEREM PROCESSADOS,QUE RGEN0218
C                              CONTEM  A  SECAO DE CHOQUE DE FISSAO,       RGEN0219
C                              (MAX  NFIS=NMAT).                           RGEN0220
C          NSIGO               (OMITIDO PARA JCODE=2)                      RGEN0221
C                              NUMERO DE  SECOES DE CHOQUE  DE  REFERENCIA RGEN0222
C                              #BACKGROUND# (SIGMA-ZERO) .                 RGEN0223
C                              OS VALORES MAXIMOS PERMITIDOS SAO:          RGEN0224
C                                NSIGO = 7, PARA JCODE=1   E               RGEN0225
C                                NSIGO = 8, PARA AS DEMAIS OPCOES.         RGEN0226
C          NT                  (OMITIDO PARA JCODE<3)                      RGEN0227
C                              NUMERO DE TEMPERATURAS, (MAX 6).            RGEN0228
C          NPN                 (OMITIDO PARA JCODE<3)                      RGEN0229
C                              ORDEM DE LEGENDRE+1 - (MAX 5).              RGEN0230
C          NWD                 (OMITIDO PARA JCODE=2)                      RGEN0231
C                              NUMERO DE CARTOES COMENTARIO A SEREM FORNE- RGEN0232
C                              CIDOS NO CARTAO DO TIPO 2.                  RGEN0233
C                                NWD(MAX)= 9, SOMENTE PARA JCODE=3         RGEN0234
C                                NWD     = 1, PARA AS DEMAIS OPCOES.       RGEN0235
C          NUTHG               (NECESSARIO SE JCODE=4)                     RGEN0236
C                              NUMERO  DO   GRUPO TERMICO   DE  MAIS  ALTA RGEN0237
C                              ENERGIA.                                    RGEN0238
C          IPRINT              VARIAVEL DE CONTROLE PARA A  IMPRESSAO (=1) RGEN0239
C                              OU  NAO  (=0)  DE  UMA  TABELA QUE CONTEM O RGEN0240
C                              DIMENSIONAMENTO  DAS  VARIAVEIS,  EFETUADO RGEN0241
C                              PELA ALOCACAO DINAMICA.                     RGEN0242
C        CARTAO  2             FORMATO(6A10) - (OMITIDO PARA NWD=0)        RGEN0243
C          ((TIT(I,J),         TITULO A SER DADO A BIBLIOTECA PRODUZIDA.   RGEN0244
C          I=1,6),J=1,NWD)                                                 RGEN0245
C        CARTAO  3             FORMATO(8E10.5) - (OMITIDO PARA JCODE<3)    RGEN0246
C          (T(IT),IT=1,NT)     TEMPERATURA EM GRAUS K.                     RGEN0247
C        CARTAO  4             FORMATO(8E10.5) - (OMITIDO PARA JCODE<3)    RGEN0248
C          (SIGO(IS),          VALORES DE  SECOES DE CHOQUE DE  REFERENCIA RGEN0249
C          IS=1,NSIGO)         #BACKGROUND# (SIGMA-ZERO) EM BARNS.         RGEN0250
C        CARTAO  5             FORMATO(5I5)-(OMITIDO PARA NMAT= OU >0)     RGEN0251
C          (MATD(IM),          IDENTIFICACAO  DOS  MATERIAIS, CONFORME  O  RGEN0252
C          IM=1,ABS(NMAT))     JAERI, A SEREM SUBSTITUIDOS NUMA BIBLIOTECA RGEN0253
C                              JA EXISTENTE.                               RGEN0254
C        CARTAO  6             FORMATO(A10,5I5)                            RGEN0255
C          ANAME(IM)           (NECESSARIO SE JCODE=3)                     RGEN0256
C                              NOMENCLATURA DO MATERIAL IM A SER PROCESSA- RGEN0257
C                              DO.                                         RGEN0258
C                              EX: PARA U-235, ANAME=  92-U-235.           RGEN0259
C          MAT(IM)             IDENTIFICACAO DO MATERIAL,CONFORME A ENDF/B RGEN0260
C          MCODE(IM)           (NECESSARIO SE JCODE=1)                     RGEN0261
C                              IDENTIFICACAO DO MATERIAL,CONFORME O JAERI. RGEN0262
C          MSF(IM)             (NECESSARIO SE JCODE=1)                     RGEN0263
C                              VARIAVEL DE CONTROLE INDICANDO QUAIS  VALO- RGEN0264
C                              RES DE SIGMA-ZERO  SERAO  ADOTADOS  PARA  O RGEN0265
C                              MATERIAL.                                   RGEN0266
C                               MSF = 0, 1.E10                             RGEN0267
C                               MSF = 1: 1.E10,1.E-10,1.E1,1.E2,1.E3,1.E4, RGEN0268
C                                        1.E5                              RGEN0269
C                               MSF = 2: 1.E10,1.E-10,1.E0,1.E1,1.E2,1.E3, RGEN0270
C                                        1.E4                              RGEN0271
C          IFIS(IM)            VARIAVEL  DE  CONTROLE  INDICANDO SE PARA O RGEN0272
C                              MATERIAL SERA PROCESSADA (=1)  OU  NAO (=0) RGEN0273
C                              A SECAO DE CHOQUE DE FISSAO.                RGEN0274
C          NRF5(IM)            VARIAVEL  DE  CONTROLE INDICANDO SE PARA  O RGEN0275
C                              MATERIAL SERA PROCESSADA (=1)  OU  NAO (=0) RGEN0276
C                              A  REACAO 18  DO   ARQUIVO 5  (ESPECTRO  DE RGEN0277
C                              FISSAO).                                    RGEN0278
C        CARTAO  7             FORMATO(2I5)                                RGEN0279
C          NRF3(IT,IM)         NUMERO DE REACOES DO ARQUIVO 3 DA ENDF/B  A RGEN0280
C                              SEREM PROCESSADAS.                          RGEN0281
C                              OS VALORES MAXIMOS PERMITIDOS SAO:          RGEN0282
C                                NRF3 =  8, PARA JCODE=1 E 2  :            RGEN0283
```

Card 6	Format (A10,5I5)
ANAME(IM)	(necessary if JCODE = 3) Nomenclature of the material IM to be processed. Ex: for U-235, ANAME = 92-U-235.
MAT(IM)	Identification of the material, according to ENDF/B
MCODE(IM)	(necessary if JCODE = 1) Identification of the material, according to JAERI.
MSF(IM)	(necessary if JCODE = 1) Control variable indicating which values of SIGMA-ZERO will be adopted for the material. MSF = 0, 1.E10 MSF = 1: 1.E10,1.E-10,1.E1.1.E2,1.E3,1.E4, 1.E5 MSF = 2: 1.E10,1.E-10,1.E0.1.E1,1.E2,1.E3,1.E4
IFIS(IM)	Control variable indicating whether the fission cross-section will (= 1) or will not (= 0) be processed, for the material.
NRF5(IM)	Control variable indicating whether reaction 18 from file 5 (fission spectrum) will (= 1) or will not (= 0) be processed for the material.
Card 7	Format (2I5)
NRF3(IT,IM)	Number of reactions from file 3 of ENDF/B to be processed. The maximum values permitted are: NRF3 = 8, for JCODE = 1 and 2; NRF3 = 18, for JCODE = 3 and NRF3 = 3, for JCODE = 4.
NRF6(IT,IM)	(omitted for JCODE > 2) Number of reactions from file 6 of ENDF/B to be processed - (max 8).
Card 8 (IR3(IR,IT, IM) IR=1, NRF3)	Format (16I5) - (omitted for NRF3 = 0) Identification of the reaction IR from file 3, according to ENDF/B.
Card 9 (IR6(IR,IT, IM) IR = 1,NRF6)	Format (16I5) - (omitted for NRF6 = 0) Identification of the reaction IR from file 6, according to ENDF/B.

In relation to the inelastic scattering matrix, the first and final excited states and the continuum - if they exist - must be given.

```
C                                NRF3 = 18, PARA JCODE=3       E                RGEN0284
C                                NRF3 =  3, PARA JCODE=4 .                      RGEN0285
C          NRF6(IT,IM)         (OMITIDO PARA JCODE>2)                           RGEN0286
C                              NUMERO DE REACOES DO ARQUIVO 6 DA ENDF/B  A      RGEN0287
C                              SEREM PROCESSADAS - (MAX 8).                     RGEN0288
C        CARTAO  8             FORMATO(16I5) - (OMITIDO PARA NRF3=0)            RGEN0289
C          (IR3(IR,IT,IM)      IDENTIFICACAO DA  REACAO  IR  DO ARQUIVO 3,      RGEN0290
C          IR=1,NRF3)          CONFORME A ENDF/B.                               RGEN0291
C        CARTAO  9             FORMATO(16I5) - (OMITIDO PARA NRF6=0)            RGEN0292
C          (IR6(IR,IT,IM)      IDENTIFICACAO DA  REACAO  IR  DO ARQUIVO 6,      RGEN0293
C          IR=1,NRF6)          CONFORME A ENDF/B.                               RGEN0294
C                              COM RELACAO A MATRIZ DE  ESPALHAMENTO  INE-      RGEN0295
C                              LASTICO, DEVEM SER FORNECIDOS, CASO EXISTI-      RGEN0296
C                              REM, O PRIMEIRO  E O  ULTIMO  ESTADOS EXCI-      RGEN0297
C                              TADOS E O CONTINUO.                              RGEN0298
C                                                                               RGEN0299
C        OBSERVACOES:                                                           RGEN0300
C        ************                                                           RGEN0301
C                                                                               RGEN0302
C        1) OS CARTOES  7 A 9  SAO REPETIDOS PARA CADA TEMPERATURA IT;          RGEN0303
C        2) OS CARTOES  6 A 9  SAO REPETIDOS PARA CADA MATERIAL IM;             RGEN0304
C        3) NA PREPARACAO DA BIBLIOTECA  SAO  CONSIDERADOS INTERNAMENTE         RGEN0305
C           PELO PROGRAMA, PARA                                                 RGEN0306
C             JCODE=1 ,  3 TEMPERATURAS (300, 900 E 2100K) ;                    RGEN0307
C             JCODE=2 ,  1 TEMPERATURA (300K)  E 1 SIGMA-ZERO (DILUICAO         RGEN0308
C                        INFINITA).                                             RGEN0309
C        4) A REACAO R0002 EM PROCESSADA SOMENTE SE JCODE=1.                    RGEN0310
C        5) A REACAO  R3100 (MF=3 E MT=100) DEVE SER SEMPRE REQUISITADA         RGEN0311
C           SE JCODE=1.                                                         RGEN0312
C        6) AS IDENTIFICACOES DOS MATERIAIS #MAT#, CASO NMAT > 1, DEVEM         RGEN0313
C           ESTAR NA MESMA ORDEM DOS QUE SE ENCONTRAM NA #GENDF#.               RGEN0314
C                                                                               RGEN0315
C                                                                               RGEN0316
C                                                                               RGEN0317
C      EXEMPLOS DE DADOS DE ENTRADA                                             RGEN0318
C      ****************************                                             RGEN0319
C                                                                               RGEN0320
C      SAO APRESENTADOS ABAIXO, EXEMPLOS DE  DADOS  DE  ENTRADA PARA AS         RGEN0321
C      OPCOES DE JCODE.                                                         RGEN0322
C                                                                               RGEN0323
C      1) JCODE=1                                                               RGEN0324
C            1    5   70    5    7    0    0    1    0    1                     RGEN0325
C         JUN/87 - 5 MATERIAIS                                                  RGEN0326
C           U-235   1261  925    1    1    0                                    RGEN0327
C            8    5                                                             RGEN0328
C            1    2    4   16   18  100  251  452                              RGEN0329
C            2   16   51   66   91                                              RGEN0330
C            6    1                                                             RGEN0331
C            1    2    4   16   18  100                                        RGEN0332
C            2                                                                  RGEN0333
C            6    1                                                             RGEN0334
C            1    2    4   16   18  100                                        RGEN0335
C            2                                                                  RGEN0336
C           U-238   1262  928    2    1    0                                    RGEN0337
C            8    5                                                             RGEN0338
C            1    2    4   16   18  100  251  452                              RGEN0339
C            2   16   51   76   91                                              RGEN0340
C            6    1                                                             RGEN0341
C            1    2    4   16   18  100                                        RGEN0342
C            2                                                                  RGEN0343
C            6    1                                                             RGEN0344
C            1    2    4   16   18  100                                        RGEN0345
C            2                                                                  RGEN0346
C          PU-239   1264  949    1    1    1                                    RGEN0347
C            8    5                                                             RGEN0348
C            1    2    4   16   18  100  251  452                              RGEN0349
C            2   16   51   76   91                                              RGEN0350
C            6    1                                                             RGEN0351
C            1    2    4   16   18  100                                        RGEN0352
C            2                                                                  RGEN0353
C            6    1                                                             RGEN0354
C            1    2    4   16   18  100                                        RGEN0355
C            2                                                                  RGEN0356
C          PU-240   1265  940    1    1    0                                    RGEN0357
C            8    5                                                             RGEN0358
C            1    2    4   16   18  100  251  452                              RGEN0359
C            2   16   51   62   91                                              RGEN0360
C            6    1                                                             RGEN0361
```

Observations

(1) Cards 7-9 are repeated for each temperature IT;

(2) Cards 6-9 are repeated for each material IM;

(3) In preparing the library, the following are considered internally by the program:

for JCODE = 1: 3 temperatures (300, 900 and 2100 K);
for JCODE = 2: 1 temperature (300 K) and 1 SIGMA-ZERO (infinite dilution).

(4) Reaction R0002 is processed only if JCODE = 1.

(5) Reaction R3100 (MF = 3 and MT = 100) must always be called up if JCODE = 1.

(6) The identifications of the materials ≠MAT≠, in the case where NMAT > 1, must be in the same order as those contained in the ≠GENDF≠.

Examples of input data

Presented below are examples of input data for the JCODE options.

[Translation of line RGEN0402:]

Library generated by the NJOY code - Jul. 86.

Inherent limitations to execution of the code

The variable ≠NARRAY≠ in the command ≠PARAMETER≠ command of the main program must be set equal to:

93500, for JCODE = 1;
30000, for JCODE = 2;
15000, for JCODE = 3, and
5000, for JCODE = 4.

This variable dimensions the vector ≠A≠, contained in the command ≠COMMON/AREA≠, which stores all the necessary information by means of dynamic allocation.

```
C            1     2     4    16    18   100                                RGEN0362
C            2                                                              RGEN0363
C            6     1                                                        RGEN0364
C            1     2     4    16    18   100                                RGEN0365
C            2                                                              RGEN0366
C          PU-241   1266   941     1     1     0                            RGEN0367
C            8     5                                                        RGEN0368
C            1     2     4    16    18   100   251   452                   RGEN0369
C            2    16    51    65    91                                      RGEN0370
C            6     1                                                        RGEN0371
C            1     2     4    16    18   100                                RGEN0372
C            2                                                              RGEN0373
C            6     1                                                        RGEN0374
C            1     2     4    16    18   100                                RGEN0375
C            2                                                              RGEN0376
C                                                                           RGEN0377
C      2) JCODE=2                                                           RGEN0378
C            2     1    70     0     0     0     0     0     0     0        RGEN0379
C          SM-147   9806   940     0     0     0                            RGEN0380
C            5     5                                                        RGEN0381
C            1     2     4    16   251                                      RGEN0382
C            2    16    51    64    91                                      RGEN0383
C                                                                           RGEN0384
C      3) JCODE=3                                                           RGEN0385
C            3     1   620     0     1     1     1     7     0     0        RGEN0386
C         THIS MATERIAL HAS BEEN PROCESSED, AT CTA/IEAV, IN A COMPUTER     RGEN0387
C         CDC 170/750, JUL/82, BY NJOY (10/81-2), WITH A FRACTIONAL        RGEN0388
C         RECONSTRUCTION TOLERANCE OF 0.005, UTILIZING THE ENOF/8-V,       RGEN0389
C         MOD 1, DOSIMETRY LIBRARY, TO PREPARE 620 GROUP (SAND-II          RGEN0390
C         STRUCTURE) GROUP AVERAGES FOR UNSHIELDED, COLD (0 KELVIN)        RGEN0391
C         AND FLAT WEIGHTED.                                               RGEN0392
C         ALL CROSS SECTIONS ARE GIVEN IN FILE 3.                          RGEN0393
C           0.                                                             RGEN0394
C             1.E10                                                        RGEN0395
C         27-CO-59  6327     0     0     0     0                           RGEN0396
C            3     0                                                        RGEN0397
C           16   102   107                                                  RGEN0398
C                                                                           RGEN0399
C      4) JCODE=4                                                           RGEN0400
C            4     2    83     2     1     1     1     1    30     0        RGEN0401
C         BIBLIOTECA GERADA PELO CODIGO NJOY - JUL/86                      RGEN0402
C           0.                                                             RGEN0403
C             1.E10                                                        RGEN0404
C            U -235 1261     0     0     1     0                           RGEN0405
C            3     0                                                        RGEN0406
C            2    18   102                                                  RGEN0407
C            U -238 1262     0     0     1     0                           RGEN0408
C            3     0                                                        RGEN0409
C            2    18   102                                                  RGEN0410
C                                                                           RGEN0411
C                                                                           RGEN0412
C                                                                           RGEN0413
C      LIMITACOES INERENTES A EXECUCAO DO CODIGO                            RGEN0414
C      =========================================                            RGEN0415
C                                                                           RGEN0416
C      A VARIAVEL #NARRAY# NO COMANDO #PARAMETER# DO PROGRAMA PRINCIPAL     RGEN0417
C      DEVE SER IGUALADA A :                                                RGEN0418
C                              93500 ,  PARA JCODE=1 ;                      RGEN0419
C                              30000 ,  PARA JCODE=2 ;                      RGEN0420
C                              15000 ,  PARA JCODE=3 E                      RGEN0421
C                               5000 ,  PARA JCODE=4 .                      RGEN0422
C      ESTA  VARIAVEL  DIMENSIONA  O  VETOR  #A#  , CONTIDO NO  COMANDO     RGEN0423
C      #COMMON/AREA#,   QUE  ARMAZENA  TODAS AS INFORMACOES NECESSARIAS     RGEN0424
C      ATRAVES DA ALOCACAO DINAMICA.                                        RGEN0425
C                                                                           RGEN0426
C                                                                           RGEN0427
C                                                                           RGEN0428
C      CARTOES DE CONTROLE PARA A EXECUCAO                                  RGEN0429
C      ===================================                                  RGEN0430
C                                                                           RGEN0431
C         JOB,T300,SC=I2. SUBMIT DO CODIGO RGENDF.                          RGEN0432
C         USER,*******,******.                                              RGEN0433
C         CHARGE,***,*****.                                                 RGEN0434
C         GET,RGENDF.                                                       RGEN0435
C         FTN5,I=RGENDF,L=0,OPT=2.                                          RGEN0436
C         *  BIBLIOTECA PRODUZIDA POR NJOY.                                 RGEN0437
C         ATTACH,TAPE1.                                                     RGEN0438
C         *  DADOS DE ENTRADA.                                              RGEN0439
```

Control cards for execution

```
JOB,T300,SC = I2.  Submit of the RGENDF code.
USER,*******,******.
CHARGE,***,*****.
GET,RGENDF.
FTN5,I=RGENDF, L=0, OPT=2.
* Library produced by NJOY.
ATTACH,TAPE1.
* Input data.
GET,TAPE5.
COPYSBF,TAPE5.
REWIND,TAPE5.
* Existing library to be updated (when JCODE = 1).
ATTACH,TAPE7.
* New library to be created.
PURGE,TAPE8/NA.
DEFINE,TAPE8.
* EXECUTE.
LGO,TAPE 5.
```

```
C         GET,TAPE5.                                                    RGEN0440
C         COPYSBF,TAPE5.                                                RGEN0441
C         REWIND,TAPE5.                                                 RGEN0442
C         *  BIBLIOTECA EXISTENTE A SER ATUALIZADA (CASO JCODE=1).      RGEN0443
C         ATTACH,TAPE7.                                                 RGEN0444
C         *  BIBLIOTECA NOVA A SER CRIADA.                              RGEN0445
C         PURGE,TAPE8/NA.                                               RGEN0446
C         DEFINE,TAPE8.                                                 RGEN0447
C         *  EXECUCAO                                                   RGEN0448
C         LGO,TAPE5.                                                    RGEN0449
C                                                                       RGEN0450
C                                                                       RGEN0451
C                                                                       RGEN0452
C     ***************************************************************** RGEN0453
```