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FEDGROUP - A Program System for Producing Group Constants from Evaluated Nuclear Data of Files Disseminated by IAEA

by

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C O N T E N T S

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ABSTRACT

A program system for calculating group constants from several evaluated nuclear data files has been developed. These files are distributed by the Nuclear Data Section of IAEA. Our program system - FEDGROUP - has certain advantage over the well-known similar codes such as: 1. it requires only a medium sized computer /≳ 20000 words memory/, 2. it is easily adaptable to any type of computer, 3. it is flexible to the input evaluated nuclear data file and to the output group constant file. Nowadays, FEDGROUP calculates practically all types of group constants needed for reactor physics calculations by using the most frequent representations of evaluated data.

1. GENERAL INFORMATION ON THE FEDGROUP SYSTEM

1.1 Introduction

The growing cooperation in the nuclear reactor physics calculation among the CMEA countries has necessitated in recent years, the revision of the available group constants libraries on the basis of common evaluated nuclear data sets. Using the opportunity offered by the Nuclear Data Section of IAEA it was decided to utilize the evaluated data files distributed by this organization. However, the codes processing these files to group constants were partly not available, partly not applicable under our circumstances. A new program system - FEDGROUP - has therefore been developed for this purpose. The initial work was done in Kurchatov's Institute, Moscow /computer BESM-6/ and in the Central Research Institute for Physics, Budapest /computer CDC-3300/. Recently, the program system has been installed in institutes of other CMEA countries taking part in the common nuclear reactor physics calculation program. By means of the FEDGROUP and IAEA files the construction of the new group constants libraries /of several types/ has been commenced.

Our intention with the FEDGROUP system is to process any nuclear data files to form group constant libraries. Up to now the processing of the files KEDAK, UKNDL, SOKRATOR and the Livermoore ENDL in ENDF/B format and the ENDF/B library have been elaborated. On the other hand there is a great diversity of group constants libraries. The construction of the FEDGROUP system facilitates the satisfying of any requirements concerning the group constants and library structure.

All segments of FEDGROUP are written exclusively in FORTRAN for BESM-6 /FORTRAN-CERN/ and for CDC-3300 and there is also a version for CYBER-72. As far as possible, any com-

puter dependent programming technique has been avoided or restricted to certain subroutines. Due to the dynamic programming, a fast storage of 20000 words and the simultaneous access of three files are enough to run the system.

Most of the abbreviations and notations in the program and in this report are standardized. Each is explained only once and not necessarily at its first occurrence. Therefore, at the end of this report a list of notations and abbreviations is given with reference to the place of explanation/s/.

1.2 Structure of the FEDGROUP system

The processing of evaluated nuclear data for group constants libraries is carried out in three stages which are connected to each other with special interface files.

1st stage: the evaluated data files which are generally in BCD card image format on magnetic tape are converted into a binary file with special format which is taken as a working file and called RFOD. The program transforming the file A to RFOD is called PRAFO for A. There are as many PRAFOs as formats of evaluated nuclear data files. Naturally, the different PRAFOs may use common auxiliary subroutines and their structure generally resemble each other.

2nd stage: the group constants are calculated from the evaluated data in RFOD and the results are stored on a file also having a special format and known as SFGK file. The program carrying out this task is called NEWZEB.

3rd stage: compilation of group constant libraries /BGK/ from the constants in SFGK. The program performing this task is called SERKON. Generally there are as many SERKONs as group constant libraries, however, a great part of these programs are common.

For detailed information on the interface files RFOD and SFGK see 2.1 and 4.4 respectively.

Sometimes it is convenient to use a scratch file for RFOD i.e. the first two stages can be included in one job.

1.3 Structure of the files and subroutines for data communications

A file in card image format will be read by

SUBROUTINE ARED

which inputs the next card from the file. After its call this card is found in COMMON/CROS/SJ(14) in A80 format. ARED strongly depends on the evaluated data file structure /e.g. blocking factor/. Sometimes code conversion or other transformation needs to be performed in ARED.

Related entry name: SARED. It is to be called before the first ARED activation.

The information on the unformatted interface files is stored as if placed in one large /theoretically unlimited/ FORTRAN field. Of course, on the storage /magnetic tape or disc/ this field is broken into blocks. In the choice of the length, LC, of these blocks one should consider the view points of the optimal data exchange. We consider that LC=1000 is an adequate choice.

The place of a quantity on such a file can be given either by its absolute address /AA/ or by its relative address /RA/ i.e.

AA - is the serial number of the word containing the quantity, taken from the beginning of the file,

RA - is also the serial number but taken from a given word of the file.

It is obvious that

AA = RA plus the length of the foregoing parts of the file

The I/O operations with these files are performed by

FUNCTION REB(LA,N,BF,NS1,NS2)

and

SUBROUTINE WRIB(LA,A,N,BF,NS1,NS2)

respectively, where

LA - is AA

REB - the input quantity /for integers NREB/

A - the output quantity

N - the logical number of peripheria

BF - the buffer field /length = LC/

NS1, NS2 - AA of the first and last words of the file being stored in the buffer BF /NS2-NS1=LC-1/

Before the first call of REB:NS1=1-LC and NS2=0; before the first call of WRIB: NS1=1 and NS2=LC should be taken as initial values. After each CALL of REB/WRIB: NS1 $\leq$ LA $\leq$ NS2.

It may be advantageous to change REB/WRIB when adapting the FEDGROUP to an other computer. Namely, an optimal access of storage by REB/WRIB may be important from the point of view of a FEDGROUP run. When using a sequential access one should take into account that the position of the file after REB differs from that after WRIB /with the same LA/.

To facilitate the input and output of the dimensioned quantities, the segments

SUBROUTINE $\begin{matrix}\text{REMA}\\ \text{WRIMA}\end{matrix}$(LA,M,W,N,BF,NS1,NS2)

are introduced, where

W(...) - is the field of variables underlying the I/O

M - is the length of this field

1.4 Name conventions

All names, i.e. names for materials, data types and group constant types are numerical ones.

The following conventions are accepted:

Material names

$MATN = i_{10}i_9i_8i_7i_6i_5i_4i_3i_2i_1$ /in case of an LENDL element i_4 and i_7 are omitted and all of four figures of DFN are retained/

where

- $i_3i_2i_1$ - atomic mass of the isotope, OOO for mixtures of isotopes
- i_4 - O for atoms, arbitrary for compounds
- $i_{10}i_9i_8$ - the last three figures of DFN, if it has been assigned in the original file [1]

Data type names

Generally the conventions described in [1] are accepted. Some exceptions can be found in the Table 2.2.

Group constant names may be arbitrary or may be inherited from the outgoing data type name. A further discussion of the group constant names will be given in 4.5

1.5 General form of a main program

The main program in a FEDGROUP run has a typical form:

```
PROGRAM MAIN
DIMENSION WORK(...)
<COMMONs in which for the variables initial values should
        be assigned>
L=<length of the dynamic field>
<assign the initial values to the variables in COMMON's>
```

```
CALL S1 (WORK,WORK,L)
.
.
CALL Sn (WORK,WORK,L)
STOP
END
```

WORK is the main field of dynamic programming, L is its length S1,...,Sn are leading segments of the FEDGROUP system.

The general form of a leading segment:

```
SUBROUTINE S(WORK, IWORK,L)
```

where S is an arbitrary name, IWORK is equivalent to WORK.

2. RFOD AND PRAFO

2.1 Structure of RFOD

The general scheme of RFOD is shown in the Figure 2.1 Except for the comments at the beginning of the file, each item of information is of numerical type. The RFOD is broken into structural parts. The RAs are always taken from the beginning of a structural part.

Table of contents /ToC/ - informs us on the materials and data types included in the RFOD. This is the third structural part.

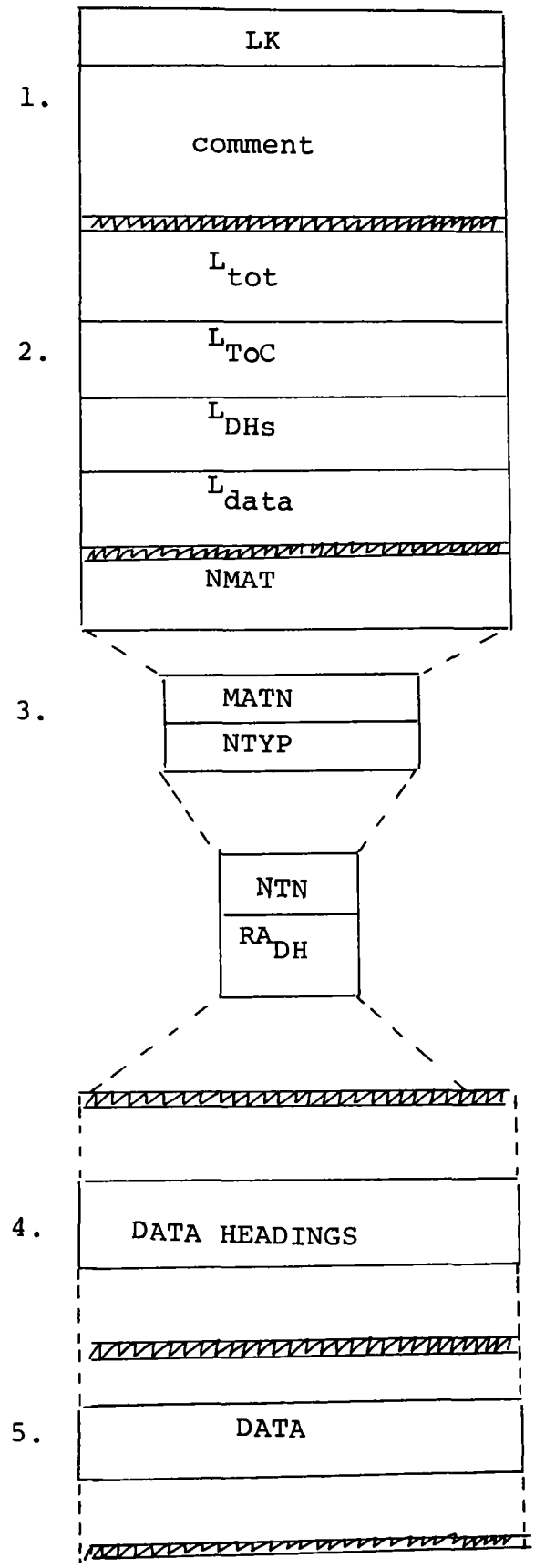
Data Heading /DH/ - informs on a data type of a given material. The fourth structural part consists of a series of data headings.

The ToC and the DHs requiring a relatively small part of storage facilitate the control of data processing.

In the fifth structural part the data are stored continuously. Information on their structure is given in the data headings.

2.2 Formats for the data headings

The first word of DH is a format type number /NTF/ this being arbitrarily assigned to a data type and it characterizes the structures of the DH and of the corresponding data set. The second word contains the length of the remaining part of the DH. In Table 2.1 the NTF introduced up to now and the corresponding DH and data structure are given. In the Table 2.2 the data types used are described.



Notations:

end of a structural part

N

loop N times

LK - length of the comment

L_{tot} - total length of the RFOD

L_{ToC}, L_{DHs} and L_{DATA} - the lengths of the ToC, DHs and the data part, respectively

NMAT - the number of materials included in the RFOD

MATN - name of the material

NTYP - number of types

NTN - the name of the type

RA_{DH} - relative address for the first word of the corresponding DH

Fig. 2.1

Structure of the RFOD file

The interpolation rules accepted in RFOD: 1-linear, 2 - logarithmic. For example if for a data set a linear-linear interpolation scheme is accepted then INTA=1 and INTF=1. The interpolation numbers are assigned by means of the segments

$$\text{SUBROUTINE } \begin{matrix}\text{INTR}\\ \text{INTW}\end{matrix}\left(\text{NTN,NTF,}\begin{matrix}\text{INTA,}\\ \text{INTW,}\end{matrix}\begin{matrix}\text{INTF}\\ \text{NW,L}\end{matrix}\right)$$

2.3 The general scheme of a PRAFO

The general scheme of the work of any PRAFO is shown on the flow-diagram of the Fig. 2.2.

The task of a PRAFO is generally simply the rearrangement of the data, however, there may be exceptions. For example if different interpolation schemes are given in different energy intervals for certain data types then the data set should be converted into one interpolation scheme at the cost of enlarging the number of energy points. The different handling of threshold reactions in the vicinity of the threshold in different files also requires a little change in the data set. Namely, if the first point in the data set is the first non-zero cross-section value then two points below the threshold with zero cross-section values should be added in order to ensure zero group averaged cross-section below the threshold. As it is seen from these examples some inconvenient deviations in the data representation need to be corrected in the PRAFO stage.

While processing the evaluated data file to RFOD the checking and correcting of the cards may be required. Therefore, after each CALL ARED a CALL ERTAPE(N) is proceeded, where N will refer to the place of the above statements. ERTAPE is programmed according to necessity.

Table 2.1 Formats of Data Headings

NTF	NL	CONTENT	Data structure
1	5	NDAT,NAC,NFC,INTA,INTF	ARG(NDAT), FUN(NDAT)
2 or 3	5	NDAT,NAC,NFC,NFF,INTA	ARG(NDAT), FUN(NFF,NDAT)
5	9	NF,NDAT1,NDAT2,NAC1, NAC2,NFC, INTAL,INTA2, INTF	ARG1(NDAT1), ARG2(NDAT2), FUN(NF,NDAT1,NDAT2)
10	N	N real numbers	-
11	2+NFN* (NW+5)	NW,NFN,((FP(J,I),J=1,NW) $NDAT_I$,$NAC_I$$NFC_I$,$INTA_I$, $INTF_I$,I=1,NFN)	ARG($NDAT_I$), FUN($NDAT_I$)
20	3	NDAT,NAC,NA	DAT(NA,NDAT)
21	2+MW+NFN* (NW+5)	NW,($INTW_I$, I=1,NW), NFN, (($FP(J,I)$,J=1,NW ,$NDAT_I$, NAC_I,NFC_I,$INTA_I$,$INTF_I$, I=1,NFN)	ARG($NDAT_I$), FUN($NDAT_I$)

Notations

NL - length of the remaining part of DH
NDAT - length of the data set
NAC - RA for the beginning of the argument vector
NFC - RA for the beginning of the function vector
INTA,INTF, and INTW - flag for the interpolation rule for argument, function and parameters, respectively
NW - the number of parameters
NA - the number of data in one set

Table 2.1 /cont./

NFN - the number of combinations of parameters
FP(...)-the values of parameters
ARG(...) - values of argument
FUN(...) - values of function

Table 2.2 Data types which can be processed by FEDGROUP

NTF=1

NTN	argument	function
1001	energy	σ_t - total cross-section
1002	energy	σ_s - elastic scattering cross-section
1003	energy	σ_x - non-elastic scattering cross-section
1004	energy	σ_{in} - inelastic scattering cross-section
1016	energy	σ_{2n} - cross-section (n,2n)
1017	energy	σ_{3n} - cross-section (n,3n)
1018	energy	σ_f - fission cross-section
1022	energy	- cross-section (n,n'α)
1023	energy	- cross-section (n,n'3α)
1024	energy	- cross-section (n,2nα)
1025	energy	- cross-section (n,3nα)
1101	energy	σ_a - absorption cross-section
1028	energy	- cross-section (n,n'p)
1102	energy	- cross-section (n,γ)
1103	energy	- cross-section (n,p)
1104	energy	- cross-section (n,d)
1105	energy	- cross-section (n,H^3)
1106	energy	- cross-section (n,He^3)

Table 2.2. /cont./

NTN	argument	function
1107	energy	- cross-section (n,α)
1108	energy	- cross-section (n,2α)
1201	energy	σ_{tr} - transport cross-section
1206	energy	η - $\nu\sigma_f/\sigma$
1207	energy	α - σ_a/σ_f
1251	energy	μ - average cosine of scattering in laboratory system
1455	energy	ν_p - prompt neutron yield by fission
1461	energy	χ_p - prompt neutron fission spectrum
1462	energy	χ_d - delayed neutron fission spectrum
4018	energy	ν - neutron yield by fission

NTF = 2 or 3

2002	energy	coefficients of the Legendre polynomials expansion in centre-of-mass system NTF = 2 or in laboratory system NTF = 3

NTF = 5

300	E_1, E_2	- moments for inelastic transfer cross-sections
200	α, β	$S(\alpha,\beta)$ - inelastic scattering function in thermal region

Table 2.2. /cont./

NTF = 10

NTN	NL	Content
458	3	A - atomic mass, Z- order of atom, I - nuclear spin in the ground state
459	3	$\lambda\sqrt{E}$ - reduced wave lenght, R - nuclear radius,
5154	3	E_b - binding energy of the last neutron average level density, a and $2\sigma^2$ constants for statistical theory

NTF = 11

NTN	parameters	argument	function
1005	threshold energy	energy	inelastic scattering cross-sections for excitation levels

NTF = 20

NTN	NA	data in one set
460	2	1. Isotopic mass 2. Abundance /%/
457	4	ν_o, ν_1, ν_2, ν_3 where $\nu = \sum_{i=0}^{3} \nu_i E_i$
5152	11	1. E_r - resonance energy 2. ℓ - orbital angular momentum 3. J - compound nucleus spin 4. g = (2*J+1)/ 2*(2*I+1)) 5. Γ - total width 6. Γ_n - neutron width 7. Γ_γ - radiation width 8. Γ_f - fission width 9. Γ_p - width for (n,p) 10. Γ_α - width for (n,α) 11. $\Gamma_{n'}$ - width for (n,n')

Table 2.2 /cont./
NTF = 20

NTN	NA	data in one set
5153	8	1. ℓ 2. J 3. $\bar{\Gamma}_\gamma$ - average radiation width 4. $\bar{D}$ - average level density 5. Γ_n^o - average reduced neutron width 6. $\Gamma_n^o/\bar{D}$ 7. ν_f - number of fission channels 8. ν_n - number of neutron channels
5155	11	1. Energy 2. ℓ 3. J 4. ν_f 5. $\bar{\Gamma}_f$ 6. $\bar{\Gamma}_\gamma$ 7. $\bar{\Gamma}_n$ - average neutron width 8. S_f 9. S_j statistical fluctuation factors 10. R_f 11. R_j strength functions

NTF = 21

NTN	parameters	argument	function
2002	energy	cosine of scattering angle	angular distributions /in center-of-mass system/

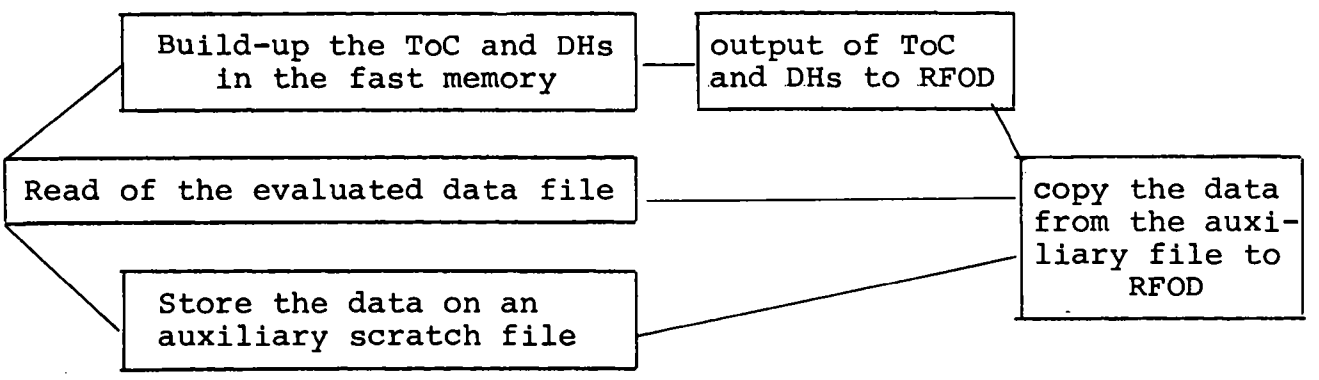


Fig. 2.2
General scheme of work of a PRAFO

The data type names and the corresponding NTF-s are generally assigned by a dictionary subroutine to be activated when a data type is being processed. When a type is not required to be processed then NTF = 0 is assigned. In this case the data type will be skipped and in the ToC of RFOD zero is assigned to the RA of the corresponding DH and, of course, no DH is introduced for this type.

The dictionary subroutine - its name may be different from file to file - contains either a tabulations with type names /names on the file and in the RFOD/ and NTFs or the assigment is performed by means of punched card input. Generally, the first alternative is preferred /in order to make the input as simple as possible/ and the punched card input is used only for a slight modification of the standard tabulation.

Generally, the evaluated data file is processed in a strict sequential order. Thus, the order of materials and data types on RFOD is the same as in the outgoing evaluated file. However, in the case of a very complicated file the practicability of a non-sequential processing is not excluded.

In the descriptions of the evaluated files [1,2,3,4] more data types with different formats are specified than is necessary for the group constant calculation. Often no data in a certain format specification are given or the data sets are obviously unimportant. /E.g. angular distribution for the inelastic scattering, which generally can be taken as being isotropic./ Therefore, there is little point in making much effort to program the processing of all specified data types. Often, in the case of a given data set, and "ad-hoc" programmed PRAFO is the quickest way to an RFOD, which is adequate for further processing.

A PRAFO may be fully automated or may be user-controlled. The full automation means that the scanning of the file and the building of the ToC and DHs require from the user only a material identifier and information on the types to be processed /or not to be processed/. In the case of a user control-

led PRAFO the ToC and the DHs are partly given by the user /by means of card input or by special program segments/ and the scanning may also require information from outside.

The required length of the dynamical field in a PRAFO run can be estimated by

$$L=2*LC+L2+L3+NDAT_{max},$$

where L2 and L3 are the length of ToC and the DHs, respectively. $NDAT_{max}$ is the maximal length of the processed data vectors.

2.4 PRAFOs for particular evaluated data files

2.4.1 KEDAK file

KEDAK is one of the simplest evaluated data files, thus its PRAFO is fully automated. The name of the leading segment is KEDAK. All card input operations are included in the leading segment and are described in Table 2.3. The initial values of the variables in COMMONs are given in Table 2.4. The dictionary segment is

SUBROUTINE SLOV(NTYP,NW,NPOT,KPOT).

where

NTYP - the number of types

KPOT - the number of modifications in the tabulation

	Before CALL	After CALL
NW(2*I-1)	name of the types in the original files	name on the RFOD
NW(2*I)	arbitrary	NTF
NPOT(1,J)	NAME1	
NPOT(2,J)	NAME2	
NPOT(3,J)	NTF	

I=1,...NTYP; J=1,...KPOT

The standard tabulation is given in Table 2.5a. This may be changed by card input.

Table 2.3 Card input of the PRAFO for KEDAK and UKNDL

Format	I/O list	Multiplicity	Condition	Remarks
3I4	NF,N,NSF1			
I6	LK			
12A6 10A8	comment	(LK-1)/12+1 (LK-1)/9 +1		BESM-6 CDC-3300
2I4	NMAT,KPOT			
3I6	NAME1,NAME2,NTF	KPOT	KPOT>0	
3I12	NAME,MAD1,MAD2	NMAT		
I12	MAD	MAD2-MAD1	MAD1>0	

Notations:

NF,N,NSF1 - logical number of the evaluated file, of the RFOD to be created and of the auxiliary scratch file, respectively

NAME1,NAME2 - the name of the type on the evaluated file and on the RFOD, respectively

MAD1, MAD2 - first and last types between which the types with identical argument vector can be found

MAD - the name of the type giving the argument to this type. If MAD=0 then its own argument vector is used.

Remark

The materials should be given in the same order as they appear on the outgoing evaluated data file

Table 2.4 COMMONs in the PRAFO for KEDAK and for UK file

Name of COMMON	length	Variables
CROS	14	SJ(14)- one card from the evaluated file
LCLCLC	1	LC* - length of the buffer
PEIF	6	NIN,NOUT* - logical number of card input and printed output, respectively NF - logical number of the evaluated file NSF1 - logical number of the auxiliary file NSF2 - no significance N - logical number of RFOD
UKKE	1	KU = {1 UK file 0 for KEDAK *

*value to be assigned in the main program or in BLOCK DATA segment

2.4.2 UK_file

The PRAFO for the UK file is also automated though not all specified data types can be fully processed. The omitted data types are generally unimportant from the point of view of group constants. The name of the leading segment is UKNDL. It controls all card input which is essentially the same as that for KEDAK. KEDAK and UKNDL use the same dictionary subroutine, and the standard tabulation is given by the Table 2.5b.

2.4.3 SOKRATOR_file

The SOKRATOR is a very complicated file. Its most inconvenient feature is that the pointwise cross-section and resonance parameters are included in the same data type. FEDGROUP always processes the pointwise cross-sections separately from the resonance parameters, which agrees well with the construction of the other evaluated data files. In addition, the intervals of different representations partly overlap.

Table 2.5a Standard dictionary tabulation for KEDAK

NAME1	NAME2	NTF	NAME1	NAME2	NTF	NAME1	NAME2	NTF
14580	458	10	14590	459	10	14600	460	20
14570	457	20	14560	3019	20	21520	5152	20
21530	5153	20	21540	5154	10	21550	5155	10
30010	1001	1	30020	1002	1	30030	1003	1
30040	1004	1	30050	1005	11	30160	1016	1
40022	2002	21	54610	3018	21	30170	1017	1
30190	1018	1	30220	1022	1	30230	1023	1
30240	1024	1	30250	1025	1	30270	1101	1
30280	1028	1	3029	1029	1	31020	1102	1
31030	1103	1	31040	1104	1	31050	1105	1
31060	1106	1	31070	1107	1	31080	1108	1
32010	1201	1	32060	1206	1	32070	1207	1
32510	1251	1	34520	4018	1	34550	1455	1
43610	1461	1	34620	1462	1	50040	3015	0
50160	3016	0						

Table 2.5b Standard dictionary tabulation for UK file

NAME1	NAME2	NTF
1000+n	1000+n n=1 ÷ 4, 16 ÷ 251	1
1000+n	1005 n=5 ÷ 15	11
2002	2002	21

There are very many formats specified in SOKRATOR [4]. In the particular SOKRATOR files which are at present at our disposal /U238 and Pu239/, only a small part of the possible representations is used. Therefore, the idea of a general PRAFO for SOKRATOR has been given up.

The work of the PRAFO for SOKRATOR U238 is user-controlled by means of card input. In this file, for example there are two overlapping intervals for resolved resonances. Because of this and other inconveniences it has been found that an automated processing would be very complicated.

In the case of SOKRATOR Pu239, the PRAFO is fitted to the file therefore no control from card input is necessary.

After the apparance of new SOKRATOR files the possibility of a more general PRAFO will be considered. It is hoped that in the future the SOKRATOR files will be simplified to make processing more convenient.

The name of the leading segment is always SOKRAT.

2.4.4 PRAFO for ENDF/B

PRAFO for ENDF/B is also developed [5]. Here it has to be taken into account that in RFOD for a data type only one interplation rule can be specified. This may require the enlargement of the number of energy points in certain intervals in order to get a data set for which one interpolation rule can be applied in the whole energy region. It seems that a PRAFO for ENDF/B can be fully automated. The name of the leading segment is ENDF. The input is described in Table 2.6.

Table 2.6 Card input of the PRAFO for ENDF/B

Format	I/O list	Multiplicity
3I4	NF,N,NSF1	
I4	LK	
12A6	Comment	(LK-1)/12+1
I4	NMAT	
3I12	NAME, MAD1, MAD2	NMAT

2.4.5 PRAFO for the Livermoore Evaluated Nuclear Data Library /LENDL/

Recently, the LENDL file in ENDF/B format has become available. The data representation and format have the following restriction:

1. no resonance parameters are given
2. only one interpolation rule is used in the whole energy interval
3. all angular distributions are given pointwise and in centre-of-mass system.

The PRAFO for LENDL files is therefore rather simple and fully automated. Its input is given in Table 2.7. The name of the leading segment is LENDL.

2.4.6 THFIL file

The program NEWRAS [6] calculates the inelastic scattering matrices or scattering law for thermal neutrons. The unformatted resulting file is known as THFIL. Its structure is described in the Table 2.8. The PRAFO for THFIL is fully automated and the card input is described in Table 2.9. The name of the leading segment is THPRAF.

Table 2.7 Card input of the PRAFO for LENDL

Format	Multiplicity	I/O list with explanation
3I4		N,NRF,NAUX - the logical number of the evaluated file, RFOD and an auxiliary file, respectively
3I4		LK, NMAT, LM - upper limit to the length of ToC
10A8	(LK-1)/10+1	comment
2I4	for all materials	NAM - the name of the material /DFN/ on the evaluated file NTYP
4I4	for all types and materials	NF, NS - file and section number, respectively NTF

Table 2.8

THFIL consists of unformatted FORTRAN records.

The general form of the I/O list is:

NM1, NM2, T, N,(W(I), I=1,N)

First record for one material /field W is equivalent to IW/:

NM1, NM2 - name of the material /Hollerith/

T - temperature

IW(1) =NFM - number of momenta

IW(2) =ND1 - number of energy points E_1

IW(3) =ND2 - number of energy points E_2

W(I+3), I=1,ND1 - outgoing energies E_1

W(I+3+ND1), I=1,ND2 - end energies E_2

The I+1 -th records for one material: i=1,ND1

NAME1=8HCONT

NAME2 and T are arbitrary

N=ND2*NFM

W(N) → SIGM(NFM,ND2) → $\sigma_m(E_1^i \to E_2^j)$ m=1,NFM, j=1,ND2

Table 2.9 Input for THPRAF

Format	Multiplicity	List
3I4		NTH,NRT,NSEG - logical number of THFIL, RFOD and the auxiliary file, respectively
LK		LK, NMAT
12A6 9A8	(LK-1)/12+1 (LK-1)/ 9+1	comment
2A8, 2I10 E12.5 I4	for each material	NAME1, NAME2 INE - numerical name of material on RFOD INT - type name on RFOD T - temperature IFO { = 0 if after read of THFIL a rewind is necessary ≠ 0 otherwise

2.5 Auxiliary programs for RFODs

2.5.1 Combining two RFODs

The program LUNION combines two RFODs in a third one. The first RFOD will be completely included. From the second RFOD the data of the materials specified by input will be copied. The input of the program given in Table 2.10.

2.5.2 Print out, copy etc. of an RFOD

There are some ad-hoc programs which may print out a specified part of an RFOD or partly copy it.

The print out of an RFOD is generally required for testing of the work of a PRAFO.

Table 2.10 Input for LUNION

Format	I/O list	explanation	remarks
3I12	L1,L2,LRES	Logical numbers of the first, second an the resulting RFOD	
I20	LC	buffer length	
I20	MATN	name of material to be included from the second RFOD	for each material till MATN $\leq$ 0
I40	LKRES	length of comment of the resulting RFOD	
9A8	comment		

A program partly copying an RFOD has the same principal scheme as that of a PRAFO.

Because of their ad-hoc character no details will be given about these programs.

2.6 Diagnostics of a PRAFO

If the dynamic field overflows, generally,a message

"REQUIRED LENGTH <n> GREATER THAN m THE EXECUTION IS TERMINATED AT PLACE <k>"

is usually printed out. However, the protection from the dynamical field overflow is not perfect,therefore, at any abnormal termination this is the first error to be suspected.

If the required material is not included in the file then the tape is scanned till its end and a system error massage may be given.

3. NUMERICAL METHODS FOR GROUP CONSTANT CALCULATIONS

3.1 Method of numerical integration

The most important group constant is the group averaged cross-section defined by the formula

$$\langle\sigma\rangle_i = \frac{\int_{Ei+1}^{E_i} dE\sigma(E)F(E)}{\int_{E_{i+1}}^{Ei} dE\ F(E)} \qquad /3.1.1/$$

where $\sigma(E)$ and $F(E)$ may be given either pointwise or by analytic functions.

In the first case set $\sigma(E)$ be given in the point E_j, then

$$\sigma(E) = f_o^j(E,\ E_j,\ E_{j+1},\ \sigma_j,\ \sigma_{j+1}) \qquad /3.1.2/$$

where $\sigma_j = \sigma(E_j)$ and f^j denotes a certain interpolation rule. Thus the integral in the numerator of /3.1.1/ is changed to

$$\sum_{j=1}^{N-1} \int_{E_{j+1}}^{E_j} dE\ f_\sigma^j \cdot F(E) \qquad /3.1.3/$$

If $F(E)$ is given by a formula then the integrals in /3.1.3/ may be calculated either analytically or by Romberg's procedure which is outlined below.

If $F(E)$ is given in the points E_ℓ then

$$F(E) = g_F^\ell(E,\ E_\ell,\ E_{\ell+1},\ F_\ell,\ F_{\ell+1})$$

where $F_\ell = F(E_\ell)$ and g_F denotes a certain interpolation rule.

The integral

$$\int_{E_a}^{E_b} dE\ f^j\ g_F^\ell$$

where $E_a = \max(E_{\ell+1}, E_{j+1})$, $E_b = \min(E_j, E_\ell)$

can obviously be analytically calculated.

If $\sigma(E)$ is given by a formula then for the evaluation of integral /3.1.1/ Romberg's procedure is used.

To put it briefly the Romberg's procedure is the following.

Let

$$I = \int_a^b dx f(x)$$

This integral is approximated by

$$I_{on} = \frac{1}{2}(f(a) + f(b)) + \sum_{k=1}^{2^n-1} f(x_N^n)\Delta x_n$$

where

$$\Delta x_n = \frac{b-a}{2^n}$$

and

$$x_k^n = a + k \cdot \Delta x_n$$

Evidently

$$I_{o,n+1} = 0.5 \times I_{o,n} + \Delta x_{n+1} \sum_{K=1,3\ldots}^{2^{n+1}-1} f(x_k^{n+1})$$

Taking the following recurrence relation

$$I_{mn} = \frac{2^{2m} I_{m-1,n} - I_{m-1,n-1}}{2^{2m} - 1}$$

it is easy to show that $|I-I_{mn}| \sim (\Delta x_n)^m$, i.e. the best approximation of I is I_{nn} at a given n. The criterion of the convergence is

$$\left| 1 - I_{n-1,n-1}/I_{nn} \right| \leq \varepsilon$$

The convergence is fast enough if $f(x)$ is a smooth function. In the case of peaks and discontinuities /e.g. resonances/ the interval /a,b/ should be divided into sub-intervals and the points of peaks and discontinuities should be the boundaries of the subintervals. However, this cannot be fully carried out in every case.Namely, there can be sub-intervals with negligible contribution but spoiling the convergence. In order to save computer time, an upper limit for n /NUJM/ is introduced. On reaching this limit an error message "NO CONVERGENCE IN ....." will be given. NUJM and the required accuracy ε are specified by card input. It is generally observed that an NUJM ≥ 4 in all cases gives a satisfying level of accuracy, disregarding the above error message.

The subroutine package evaluating the integral /3.1.1/ consists of the following segments.

FUNCTION FXINT(EP, EM, SGN, ES, FL, ER, NP,
NDAT, INTA, INTF)

Calculates

$$\int_{EM}^{EP} dE \ (E)F(E)dE$$

where

SGN(...)→σ(E), FL(...)→F(E), ES(...) ER(...)

FUNCTION SINT(SG1, SG2, E1, E2, INTA, INTF,
ER, FL, NP)

calculates $\int_{E_1}^{E_2} f_\sigma(E, SG1, SG2, E1, E2)F(E)dE$

FUNCTION CRINT(EP,EM,FUN,APAR,LPAR)

calculates $\int_{EP}^{EM} \phi(E,par)dE$ by means of Romberg's procedure.

$\phi(E,par) \rightarrow$ FUN and the field APAR contains LPAR number of parameters.

In connection with the numerical integration the auxiliary segment

SUBROUTINE ZWIN(NDAT,EP,EM,ES,J2,J1)

is used. It determined J1, J2 so that

ES(J2) < EM<.....>EP $\leq$ ES(J1).

3.2 Cross-sections in the resonance energy region

The cross-sections from the resolved resonance parameters are calculated by means of the multilevel Breit-Wigner formula: [7]

$$\sigma_t = \sum_{\ell,r} \sigma_t^{\ell,r}(E)T$$

$$\sigma_x = \sum_{\ell,r} \sigma_x^{\ell,r}(E,T)$$

where

$$\sigma_t^{\ell,r}(E) = 4\pi(2\ell+1)\lambda^2\sin^2\delta_\ell + {}_r\sigma_{oc}(\psi_r\cos 2\delta_\ell + \chi_r\sin 2\delta_\ell + \psi_r\alpha_r - \chi_r\beta_r)$$

$$\sigma_x^{r,\ell}(E,T) = \sigma_{ox}\psi_r \qquad /3.2.1/$$

and

$$ {}_r\sigma_{oc} = 4\pi\lambda^2(E_r)g\frac{\Gamma_n^r}{\Gamma^r}\frac{E}{E_r}^{\ell-1/2} $$

$$ {}_r\sigma_{ox} = {}_r\sigma_{oc}\frac{\Gamma_x^r}{\Gamma^r} $$

$$ \psi(\theta,x) = \frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty} dy\ \frac{\exp(-\frac{\theta^2}{4}(x-y)^2)}{1+y^2} $$

$$ \theta = \Gamma\sqrt{\frac{A}{4kTE_r}} $$

$$ X = \frac{2(E-E_r)}{\Gamma_r} $$

$$ \delta_\ell = \frac{R}{\lambda} - \operatorname{arctg}\frac{R}{\lambda}\cdot\ell $$

$$ \alpha_r = \frac{1}{2}\sum_{s\neq r}\Gamma_{sn}(\Gamma_s+\Gamma_r)/D_{sr} $$

$$ \beta_r = \sum_{s\neq r}\Gamma_{sn}(E_s-E_r)/D_{sr} $$

$$ D_{sr} = (E_s-E_r)^2 + \frac{1}{4}(\Gamma_s+\Gamma_r)^2 $$

E_r - resonance energy
R - nuclear radius
λ - $\lambda\sqrt{E}$ = reduced neutron wavelength
ℓ - orbital angular momentum
- statistic spin-factor

If $T \to 0$ then

$$ \psi_r = \frac{1}{1+x^2} $$

$$ \chi_r = \frac{x}{1+x^2} $$

For resonances at negative resonance energies

$$r\sigma_{oc} = 4\pi\Lambda_o^2 g \frac{\Gamma_n^r}{\Gamma^r} E^{\ell-1/2} \quad (\Lambda_o = \lambda(1\ eV)).$$

In the case of resonances with statistical parameters a simpler approximation is used

$$\sigma_t^\ell(E,T) = \sigma_{oc}\ \psi \cos 2\delta_\ell$$

$$\sigma_t^\ell(E,T) = \sigma_{ox}\ \psi$$

i.e. the asymmetrical term in the total cross-section is neglected.

The average level spacing is calculated by the formula [8]

$$\bar{D} = \bar{D}^o \frac{(E_B+E)^2}{E_B^2} \exp\left(-\sqrt{89,72(E_B-E)} + \sqrt{89,72\ E_B}\right)$$

E_B – binding energy of the last neutron in the compound nucleus in MeV

E – energy in MeV

$$\Gamma_\lambda = \bar{\Gamma}_\gamma$$

and for the distribution of neutron and fission half-width a χ^2-distribution is used with the degree of freedom given in the library.

The average neutron half width is calculated from the reduced average neutron half-width by

$$\bar{\Gamma}_n = \bar{\Gamma}^o\sqrt{E}\ \left(1+\frac{\ell\lambda^2}{R^2+\lambda^2}\right)$$

for $\ell = 0,1$

Segments for resonance cross-section calculation from resolved parameters are

SUBROUTINE RESKO (RPAR,JR,NA)

NA - number of parameters for one resonances /in our case NA=13/

RPAR(NA,JR) - resonance parameters

JR - number of resonances

RPAR(1,IR), RPAR(2,IR), ... RPAR(11,IR) - are - before the CALL - the resolved parameters given in Table 2.2. After the CALL some of them will be changed:

RPAR(3,IR) = α RPAR(12,IR) = γ_r

RPAR(4,IR) = β RPAR(13,IR) = 2.*√ER/A*8.617E-5

RPAR(6,IR) = σ_{oc}

SUBROUTINE XSEC(RPAR(1,IR))

calculates the values $\sigma_{ox}\psi$ and $\sigma_{oc}(\psi\cos 2\delta + \psi\sin 2\delta)$ for a certain resonance at energy E and temperature T. The latter parameters are communicated between subroutines by the

COMMON/BLS6/E,T,A,RLAM,RR,ST,SX

where

RR - is the R nuclear radius

RLAM - $A\sqrt{E}$ - reduced wave length

ST - $\sigma_{oc}(\psi\cos 2\delta + \psi\sin 2\delta)$

SX - $\sigma_{ox}\psi$

The resonance cross-sections contributed from all resolved resonances are calculated by

SUBROUTINE RESEC(RPAR,NA,JR,SRX)

where SRX(1)→ σ_t^r , SRX(2)→ σ_s^r , SRX(3)→ σ^r , SRX(4)→ σ_f^r

SRX(5)→γ

10-10 resonances are taken into account on both sides of E.

3.3 Calculation of resonance-screened group averaged cross-sections

The resonance screened group averaged cross-sections are defined by

$$\langle\sigma_x(T,\sigma_o)\rangle^i = \frac{\int_{E_{i+1}}^{E_i} \sum_r \frac{\sigma_x^r(E,T)}{\sigma_q+\sigma_o}\,\phi(E)}{\int_{E_{i+1}}^{E_i} dE\,\frac{1}{\sigma_q+\sigma_o}\,\phi} \qquad /3.3.1/$$

where $\phi(E)$ is a smooth function and

$$\sigma_q(E,T) = \sum_r \left(\sum_x \sigma_x^r(E,T)\,(1-\gamma_r)+\gamma_r\sigma_t^r(E,T)\right)$$

x - refers to a nuclear reaction

t - refers to the total cross-section

γ_r - is a factor taking into account the finite width of resonances according to the theory of Goldstein [11].

It is calculated by means of the Forti approximation [12]:

$$\gamma_r = \begin{cases} 1-1/2\,\frac{\Gamma_r}{\alpha E_r} & \text{if} \quad \alpha \geq \frac{\Gamma_r}{E_r} \\ 1/2\,\frac{\alpha E_r}{\Gamma_r} & \text{if} \quad \alpha \leq \frac{\Gamma_r}{E_r} \end{cases}$$

where

$$\alpha = \log\left(\frac{A+1}{A-1}\right)^2$$

A group averaged value can be assigned to γ by

$$\gamma_i = \frac{\int_{E_{i+1}}^{E_i} dE\,\gamma(E)\,\sigma_x(E)\,\phi(E)}{\int_{E_{i+1}}^{E_i} dE\,\sigma_s(E)\,\phi(E)}$$

where

$$\gamma(E)\sigma_s(E) = \sum_r \gamma_r(\sigma_t^r(E,T) - \sum_x \sigma_x^r(E,T))$$

$$\sigma_s(E) = \sum_r (\sigma_t^r(E,T) - \sum \sigma_x^r(E,T))$$

As in the case of narrow resonance approximation $\gamma = 1$, γ will be calculated only then when resolved parameters are used.

If the cross-sections are given pointwise then the evaluation of formula /3.3.1/ is similar to that of the infinite dilute group averaged cross-sections i.e. the formalism given in 3.1 is used. The only difference being that instead spectrum $\frac{\phi}{\sigma_q+\sigma_o}$ should be generated and used.

If cross-sections are given by resolved resonance parameters then the integrals in /3.3.1/ are calculated in the following way. The interval (E_{i+1},E_i) is divided into sub-intervals by means of the resonance energy points and the points lying in the distance $q\Gamma$ from the peak on both sides where $q=\frac{1}{2}\sqrt{\frac{\sigma_{oc}}{\sigma_{pot}}}$. If the distance of resonances $\underline{a}$ and $\underline{b}$ is less than $q_a\Gamma_a+q_b\Gamma_b$ then the point

$$E_a + \frac{\Gamma_a(E_b-E_a)}{\Gamma_a+\Gamma_b}$$

is taken.

In each sub-interval Romberg's integration procedure is applied. In order to save computer time in every energy point only the contribution of M-M neighbouring resonances on both sides are calculated exactly. As the contribution of the remaining resonances is assumed to be slowly varying in the given sub-interval, it is calculated only at both ends of each sub-interval and within the sub-interval its values is determined by linear interpolation. We have found that even M=2 gives satisfying results.

The integration is performed by

SUBROUTINE ROMRES(RINT,LR,RPAR,NA,JR,SGT,SGS,SGI,
SIGF,NT,NSI,PL,PER,AL,AJ,AP,VEG,IT,ER,FL,SIG,WORK,LFR)

where

RINT(...) - boundaries of sub-intervals

LR - number of sub-intervals

PL,PER,AL,AJ,AP,VEG - are working fields for integration.

The segment

SUBROUTINE RESCAL(EP,EM,NA,JR,RPAR,SGT,SGS,SGI,
SGF,WORK,T,SIG,ER,FL,LFR,NSI,NT)

determines the sub-intervals and controls the calculation of the integrals /3.3.1/

T(...) the temperature values

SIG(...) the σ_o values.

In the region of unresolved resonances the interval $/E_{i+1},E_i/$ is divided into sub-intervals in which the variation of the parameters is negligible; though they are large enough to contain many resonances. As a result, the cross-sections are smoothly varying within these sub-intervals, i.e.

$$\langle\sigma_x\rangle^i = \frac{\int \sum_j F_j \Delta E_j \, \overline{\sigma_x(E_j^*)}}{\int \sum_j F_j \Delta E_j}$$

The averaged cross-sections are composed of the contribution of all resonance series $\underline{s}$ i.e.

$$\sigma_x(E_j^*,\sigma_o,T) = \sum_s \sigma_x^s(E_j^*,\sigma_o,T)$$

According to the results reported in [8]

$$\sigma_x^s(E_j^*,T,\sigma_o) = \sigma_{p,eff}^s \frac{(1+\frac{\langle\sigma_r^s\rangle}{\langle\sigma_t\rangle})\frac{\Gamma_x^s J(\theta^s,\beta^s)}{s_{\bar{D}}\cos 2\delta_\ell} - \frac{s_D\langle\sigma_x^s\rangle\langle\sigma_r^s\rangle}{\Delta\sqrt{2\pi}\langle\sigma_t\rangle^2}\varepsilon}{(1-\frac{\langle\sigma_r^s\rangle}{\langle\sigma_t\rangle})\frac{\Gamma^s J(\theta^s\ \beta^s)}{s_{\bar{D}}} + \frac{s_{\bar{D}}\langle\sigma_r^s\rangle^2}{\Delta\sqrt{2\pi}\langle\sigma_t\rangle^2}\varepsilon}$$

where /3.3.2/

$$\langle\sigma_x^s\rangle = \frac{2\pi^2}{s_{\bar{D}}}\lambda^2 g\left[\frac{\Gamma_n^s\Gamma_x^s}{\Gamma^s}\right]$$

$$\langle\sigma_r^s\rangle = \frac{2\pi^2}{s_{\bar{D}}}\lambda^2 g\Gamma_n^s\cos 2\delta_\ell$$

$$\langle\sigma_t\rangle = \sigma_o + \sigma_p + \sum_s\langle\sigma_r^s\rangle$$

$$\sigma_{p'eff} = \langle\sigma_t\rangle - \langle\sigma_r^s\rangle$$

$$\beta^s = \frac{\langle\sigma_t\rangle}{\sigma_c^s\cos 2\delta_\ell} \qquad \Delta = \sqrt{\frac{4kTE_j^*}{A}}$$

Formula /3.3.2/ takes the resonance overlapping into account. The segment for the calculation of ε /EPSI/ and the numerical method for averaging the resonance widths over the χ^2 distribution are also taken from [8].

For a series s the average cross-sections are calculated by the segment

SUBROUTINE RESCAL (EP,EM,NA,JR,RPAR,SGT,SGS,SGI,SGF,WORK, T, SIG,ER,FL,LFR,NSI, NT)

where AL → ℓ, AJ → J, NUF → ν_f, NUN → ν_n, GAM(...) - average widths, RIS - nuclear spin in the ground state.

The function $J(\theta,\beta)$ is calculated by means of FUNCTION FJ2 (TET,BET)

where θ → TET, β → BET. This segment is taken from [13].

3.4 Calculation of the inelastic transfer matrix in the fast region

In the epithermal region the inelastic scattering process is generally described by the following data types:

1. inelastic scattering cross-section for resolved excitation levels
2. inelastic scattering cross-section for unresolved excitation levels /i.e. for a continuum/
3. total inelastic cross-section.

These data are, of course, redundant: 1 and 2 or 1 and 3 are enough for the calculation of the inelastic scattering transfer matrix. If, on the evaluated data file, all of them are given then either 2 or 3 should be excluded from the RFOD.

It is assumed that the first two energy points of a level cross-section are under its threshold energy in the laboratory system, and the last energy points are the same /EZ/ for all levels. If EZ differ for different levels then that for the first level is taken as a common one. Above EZ, there is the region of unresolved inleastic scattering.

In the resolved region the inelastic energy transfer is described by

$$\sigma_{in}(E\to E') = \sum_k \sigma_{in}^k(E)\,\delta(E-E'-\langle E\rangle_k) \qquad /3.4.1/$$

where [14]

$$\langle E\rangle_k = \frac{A^2+1}{(A+1)^2}\,E - \frac{A}{A+1}\,Q_k$$

Q_k - threshold energy in the centre of mass system for the k-th level.

$$\sigma_{in}^{i\to j} = \sum_k \sigma_{in,k}^{i\to j} \qquad /3.4.2/$$

where

$$\sigma_{in,k}^{i\to j} = \begin{cases} \text{if } E_i > E_{j+1} + \langle E\rangle_k \geq E_{i+1} \text{ then} \\ \min(E_i, E_j+\langle E\rangle_k) \\ \int_{E_{j+1}+\langle E\rangle_k} \sigma_{in}^k(E)\phi(E) \Big/ \int_{E_i+1}^{E_i} dE\phi(E) \\ \text{if } E_i > E_j + \langle E\rangle_k > E_{i+1} \text{ then} \\ \int_{\max(E_{i+1},\, E_{j+1}+\langle E\rangle_k)}^{E_j+\langle E\rangle_k} \sigma_{in}^k(E)\phi(E) \Big/ \int_{E_i+1}^{E_i} dE\phi(E) \\ 0 \quad \text{otherwise} \end{cases} \qquad /3.4.3/$$

In the unresolved region the evaporation model [15] is used.

$$\sigma_{in}^{i\to j} = \int_{E_{i+1}}^{E_i} dE\phi(E)\sigma_{in}(E)P(E\to j) \Big/ \int_{E_{i+1}}^{E_i} dE\phi(E) \qquad /3.4.4/$$

where

$$P(E\to j)=\Theta^2(E)\left[e^{-\frac{E_{j+1}}{\Theta(E)}} 1 + \frac{E_{j+1}}{\Theta(E)} - 1 + \frac{E_j}{\Theta(E)} e^{-\frac{E_j}{\Theta(E)}}\right] \qquad /3.4.5/$$

$\Theta(E)$ - is the nuclear temperature. In FEDGROUP

$$\Theta(E) = \sqrt{\frac{E}{0,16A}}$$

is taken [15].

The inelastic transfer matrix for the resolved levels is calculated by

SUBROUTINE INEL (IWX,NFN,EG,ER,FL,A,NGIN,IGO, IWS,EZ,WORK,LFR,BFG)

IWX(...) - DH for the type 1005 taken from its 5th word
NGIN = NGO - NR1+1
IGO - the group containing the threshold of the first excitation level
IWS = IGO - NR1 + 2

If the total scattering cross-section is given in the unresolved region the inelastic transfer matrix is calculated by

SUBROUTINE DIV (IW4,EZ,A,EG,ER,FL,SIGI,NGIN,IGO, SIGM,WORK,LFR,BFG)

IW4(...) - DH for the type 1004
SIGI(...) - $(\langle\sigma_{in}\rangle^{i}$, i=NR1, IGO)
SIGM ... - $((\langle\sigma_{in}\rangle^{i\to j}$, j=i, NGIN), i=NR1,NR2).

If the cross-section for the unresolved levels are given the transfer matrix is calculated by

SUBROUTINE DIVUK(NDAT,NFC,INTA,A,EP,EM,IG,NGIN,EZ, SIGI,SIGM,WORK,FL,ER,EG,LFR,BFG,XARG.)

This calculates the transfer matrix elements for the group IG. NDAT,NFC,INTA,INTF belong to the cross-section for an excitation level, XARG ... are the energy points for this cross-section.

Auxiliary subroutines for the unresolved inelastic calculation WINELS,EXD,DNFAK are taken from MIGROS-2 [8].

3.5 Calculation of the inelastic transfer matrix in the thermal region

In the thermal region the inelastic transfer process can be described by

$$\sigma(E_1 \to E_2,\mu) = \sum_{\ell=0}^{L} (2\ell+1)\sigma_\ell(E_1 \to E_2)P_\ell(\mu) \qquad /3.5.1/$$

It is assumed that $\sigma_\ell(E_1 \to E_2)$ are given on the data file for a set of E_1 and E_2 and for $\ell=0,1,\ldots L$. As mentioned in 2.4.6 $\sigma_\ell(E_1 \to E_2)$ is calculated rather then stored. By means of phonon spectra they can be generated by the program NEWRAS [6].

In reactor physics calculations either the $\sigma_\ell(E_1 \to E_2)$ or its group averaged value

$$\bar{\sigma}_\ell^{i\to j} = \frac{\int_{E_{j+1}}^{E_j} dE_2\chi(E_2) \int_{E_{i+1}}^{E_i} dE_1 M(E_1)\sigma_\ell(E_1 \to E_2)}{\int_{E_{j+1}}^{E_i} dE\chi(E) \int_{E_{i+1}}^{E_i} dE M(E)} \qquad /3.5.2/$$

is required, where $M(E)$ and $\chi(E)$ are the thermal neutron spectrum and its adjoint function, respectively.

3.6 Calculation of the elastic scattering transfer matrices

3.6.1 Description of the elastic scattering transfer process

In order to get an adequate elastic group transfer matrix the angular distribution of elastic scattered neutrons as a function of ingoing neutron energy is required. Up to a

definite energy /generally 10-50 keV/ an isotropic (in the centre-of mass system) angular distribution can be taken. In this region the calculation of the elastic transfer matrix is especially simple. Over this region the angular distribution may be given as a function of the cosine of the scattering angle, μ , pointwise or by the coefficient of Legendre polynomial expansion. In the files KEDAK, UK and LENDL the first way is preferred, while in the SOKRATOR and ENDF/B files the second way is preferred. Our method of calculation is based on the pointwise representation of angular distribution, i.e. before calculation any other representation is transformed into this one. If the angular distributions are given in the laboratory system then the transformation into the centre-mass system is also performed.

Pointwise angular distribution from Legendre expansion coefficients is calculated by

SUBROUTINE LEGMU(E,IK,NDAT,NFC,INTF,MANG,NFF,EARG, XARG,FUN,WORK,LFR,BF,A)

E - energy point for which the angular distribution is required

IK $\leq$ { 1 coefficients are given in the centre-of-mass system; 2 coefficients are given in the laboratory system

EARG(...) - energy values for which the coefficients are given

XARG(...) - angle points

MANG - number of angle points

NDAT,NFC,INTF,NFF see Table 2.1 for NTF=2 or 3

FUN(...) - the calculated pointwise distribution.

3.6.2 Calculation of the elastic transfer matrix up to P_5 approximation

For the elastic transfer matrix calculation up to P_5 approximation the method developed in Module 9. of MIGROS-2 [8] is used. In this module the groups are divided into fine intervals and the elastic transfer probability from a fine interval into a group is calculated. In FEDGROUP the special case where the number of fine intervals = 1 is applied. In the present report the theory and those parts of program which have been overtaken over from MIGROS-2 are not discussed and we are referring to Chapter 8. of the report [8]. The MIGROS-2 module differs from that of the corresponding FEDGROUP mainly in the preparation of the elastic scattering data for numerical integration since FEDGROUP's RFOD differs considerably from the KEDAK's random access library. In addition FEDGROUP is able to use Legendre polynomial data in the way outlined in 3.6.1. An further deviation of the two programs is caused by the lack of the average scattering cosine data which is on most of the evaluated files apart from KEDAK. It should be foreseen that in this case no correction to the average cosine can be provided. This leads to some small changes in the subroutines performing the correction.

The segment preparing all kind of data is

```
SUBROUTINE PARANG(NS,NM,NC,EP,EM,BF,WORK,IWORK,LFR)
```

where NS(...), NM(...), NC(...) are DHs for the types 1002,1251, and 2002, respectively.

The segment preparing the angular distribution is the pointwise case is

```
SUBROUTINE REANG(IWX,EP,EM,BFG,WORK,IWORKARGM,LFR)
```

where IWX(...) - DH of the type 2002 beginning from the 3rd word

ARGM(...)- angle points

IWORK(26) - number of angular distribution in the energy interval EP,EM.

The analogous segment in the Legendre polynomial case is SUBROUTINE LEGDIS(IWX,EP,EM,WORK,IWORK,ARGM,MANG,BFR,LFR,A) where

IWX(...) - is the DH of the type 2002.

3.6.3 Calculation of Greuling-Goertzel constants for continuous slowing down

The Greuling-Goertzel continuous slowing-down model is described e.g. in [9]. The constant to be used in the equations of continuous slowing down are defined by

$$\mu_j = \int_{E_{j+1}}^{E_j} dE\phi(E)G_1^o(E) \; / \sigma_s(E) \; / \int_{E_{j+1}}^{E_j} dE\phi(E) \qquad /3.6.1a/$$

$$\xi_j = \int_{E_{j+1}}^{E_j} dE\phi(E)G_o^1(E) \; / \sigma_s(E) \; / \int_{E_{j+1}}^{E_j} dE\phi(E) \qquad /3.6.1b/$$

$$\eta_i = \int_{E_{j+1}}^{E_j} dE_\phi(E)G_1^1(E) \; / \sigma_s(E) \; / \int_{E_{j+1}}^{E_j} dE\phi(E) \qquad /3.6.1c/$$

$$\Gamma_j = \int_{E_{j+1}}^{E_j} dE\phi(E)\Lambda_o(E) \; / \int_{E_{j+1}}^{E_j} dE\phi(E) \qquad /3.6.1d/$$

$$Z_j = \int_{E_{j+1}}^{E_j} dE\phi(E)\Lambda_1(E) \; / \int_{E_{j+1}}^{E_j} dE\phi(E) \qquad /3.6.1e/$$

$$\xi_j = \xi_j \left(1 - \frac{\Lambda_o(E_j)/E_j - \Lambda_o(E_{j+1})/E_{j+1}}{E_j - E_{j+1}}\right) \qquad /3.6.1f/$$

$$H_j = \eta_j \left(1 - \frac{\Lambda_1(E_j)/E_j - \Lambda_1(E_{j+1})/E_{j+1}}{E_j - E_{j+1}}\right) \qquad /3.6.1g/$$

where

$$\lambda_i(E) = - \frac{G_i^2(E)}{G_i^1(E)}$$

$$G_i^n(E) = \frac{2\pi}{n!} \int_{-1}^{1} d\mu_c P_i(\mu_o)(\log W)^n \sigma_s(\mu_c, E) \qquad /3.6.2/$$

$$W = 1 - \frac{2A}{(A+1)^2} \quad (1 - \mu_c)$$

$$\mu_o = \sqrt{W} \left(\frac{A+1}{2} - \frac{A-1}{2W}\right)$$

$\sigma_s(\mu_c E)$ - is the angular distribution of elastically scattered neutrons in the centre-of-mass system.

Numerical integration over μ is carried out according to the trapezoidal rule.

If the scattering is isotropic then we have got explicit formulae for the above constants:

$$\mu = \frac{2}{3A}$$

$$\xi = \xi^* = \frac{(A+1)^2}{4A} \left(1 - \frac{A-1}{A+1}\right)^2 (1+q) \qquad /3.6.3a/$$

$$\eta = H = \frac{(A+1)^2}{4A} \frac{A+1}{3} 2/3 - (2/3+q)e^{-1.5q} - (A-1)(2-(2+q)e^{-q/2}) \qquad /3.6.3b/$$

$$\Gamma = -\frac{(A+1)^2}{4A}\ \frac{1}{2\xi}\ 2 - (2+2q+q^2)e^{-q} \qquad /3.6.3c/$$

$$Z = -\frac{(A+1)^2}{4A}\ \frac{1}{2\eta}\ \left|\frac{A+1}{3}\ 8/9 - (8/9+4/3q+q^2)e^{-q}\right.$$

$$\left. - (A-1)/8 - (8+4q+q^2)e^{-q/2}\right| \qquad /3.6.3d/$$

$$q = \log\left(\frac{A+1}{A-1}\right) \qquad /3.6.3e/$$

It should be noted that all scattering transfer matrix elements as well as Goertzel-Greuling constants are averaged over the same spectrum. This is not quite correct but in most of the cases seems to be a good approximation.

4. THE PRINCIPAL PROGRAM FOR GROUP CONSTANTS CALCULATION: NEWZEB

4.1 General scheme of NEWZEB

In the Fig 4.1 the flow diagram of NEWZEB is given.

Explanation

P1 - card input of the task's parameters, opening the files to be used
P2 - specification of the group system and averaging spectrum
P3 - specification of materials and types of the group constants to be calculated by card input.
P4 - input of data headings of the required types from RFOD
P5 - determination of the optimal schedule of the calculation /the optimal schedule means an optimal access of storage holding the RFOD/
P6 - one of the blocks for group constant calculation
Q1 - Is this the last type of group constants?
Q2 - Is this the last material?
Q3 - Is this the last task?

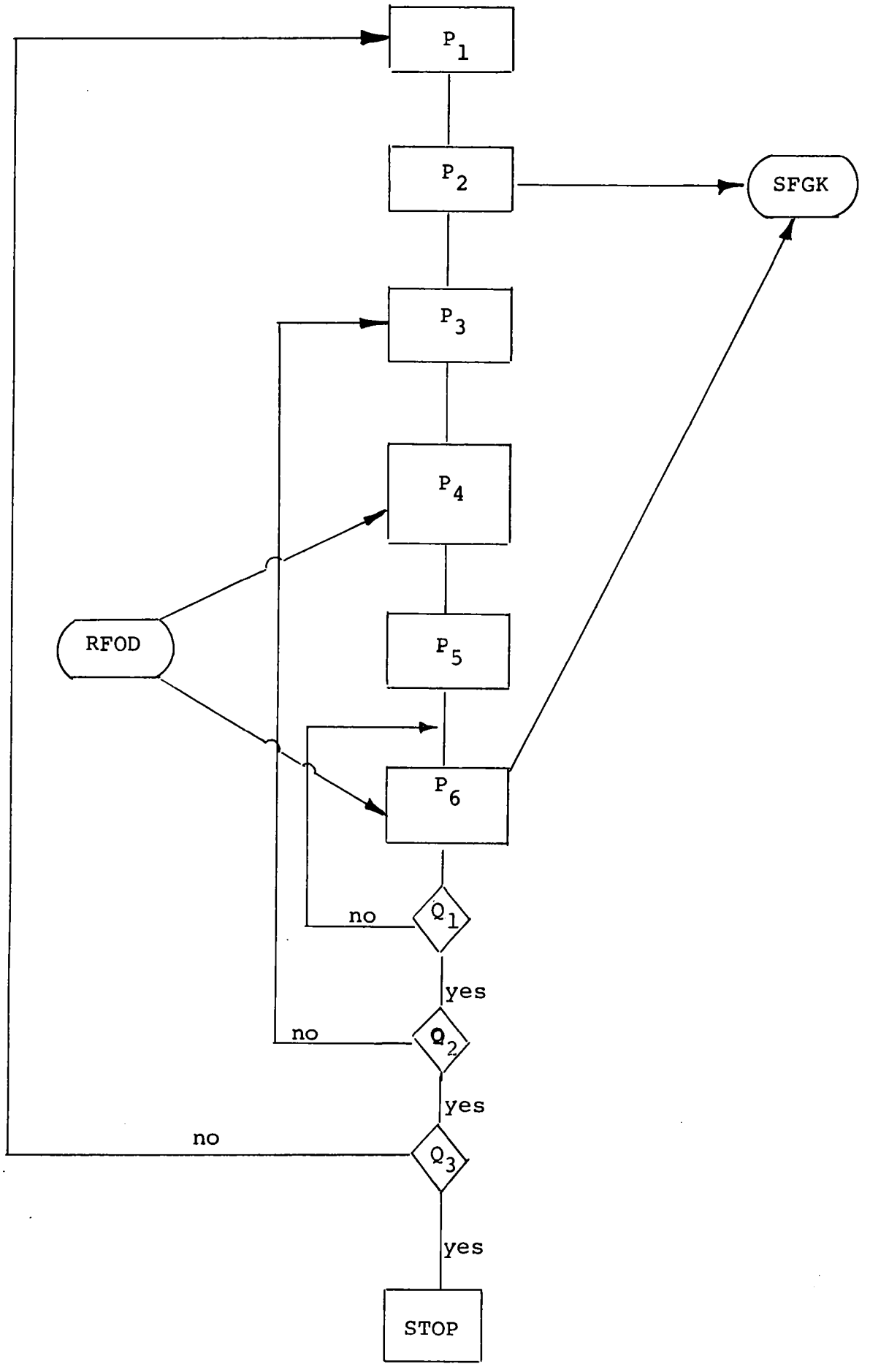
The name of the leading segment is INZEB, where P1, P2 and P3 are carried out.

P4 and P5 are carried out in

SUBROUTINE GROP (BFG, BFK, EG, MATYP, IRES, RES, WORK, LFR, ER,(FL)

where

BFG - buffer for RFOD
BFK (...) - buffer for SFGK
EG (...) - group - boundaries
ER (...) - energy points for averaging spectrum
FL (...) - averaging spectrum


P1
P2
SFGK
P3
P4
RFOD
P5
P6
no
Q1
yes
no
Q2
yes
no
Q3
yes
STOP

MATYP (...) contains information on material and types to be calculated

IRES (...) - contains information on the parameters to be used /e.g. temperature/

RES (...) - contains parameters to be used

The evaluated data types required for the calculation of a certain group constant types are specified by the

SUBROUTINE REQT (NTNAM, NFEL, NTR)

where

NTR(1) - number of types

NTR(K+1) - NTN_k

The segments performing the tasks P1-P5 are the organizing part of NEWZEB.

The place in the dynamic field required by this part is

$$L_{org} = L_{buf} + L_{par} + L_{ToC} + L_{DH}$$

where

$$L_{buf} = \begin{cases} LC \text{ is } NGL = 0 \\ 2*LC \text{ if } NGL > 0 \end{cases}$$

$$L_{par} = NGO + 3 + 2 * NP + MAX(8*NTYP_j) + MAX+(NT_j + NSI_j)$$

$NTYP_j$ is the number of types and NT_j, NSI_j, are the number of the first and second parameters for the material j, respectively.

$$L_{ToC} = MAX\left(NTYP_j + \sum_{i=1}^{NTYP_j} N^i_{req} + 2*NLTYP_j\right)$$

N^i_{req} = is the number of required nuclear data types for the calculation of the group constant type i.

$NLTYP_j$ is the number of required nuclear data types

$$L_{DH} = MAX\left(\sum_{i=1}^{NLTYP_j} N^k_{pass}\right)$$

N^i_{pass} - length of the DH for the nuclear data type k.

It can be seen that the corresponding ToC and DHs are retained in the core memory while calculating the group constants for a material.

The required length of the dynamic field in the calculation of group constant i for material j is

$$L_{ji} = L_{org} + L_{block_i}$$

L_{block_i} - the length required by the block i. This will be discussed in 4.5.

4.2 Specification of the group structure and the averaging spectrum

The group system for which the constants are to be calculated may be arbitrary. The group boundaries should be given in descending order. There are four possibilities for specifying the group boundaries:

1./ Built-in standard systems. In the present version the group system Grace [9] /key-number=0/ and the 26-group Bondarenko system /key-number=-2/ are built-in. The standard group boundaries are assigned by the segment

SUBROUTINE DEFGR (NGO,EG)

Before CALL NGO = the key number, after CALL NGO = number of groups.

2./ System specified by card input /key-number = number of groups/

3./ System created by dividing a coarse-group system into fine groups /key-number = -1/. The coarse group system and the number of fine groups/ coarse group are specified by card input.

4./ Arbitrary group system determined by a specially written program segment /key-number = arbitrary/. In connection with

the group boundaries the standard output segment VIVOD is called. Through the free subroutine VIFORM, which is called by VIVOD the group boundaries can be arbitrary changed by a program part to be written by the user.

There are two possibilities for specifying the averaging spectrum.

1./ Spectrum given by formula /key-number=1/

The following segments are related to the spectrum:

FUNCTION PHI(E)

This gives the value F(E).

FUNCTION PSI(E1, E2)

This gives the value $\int_{E_1}^{E_2} dEF(E)$

FUNCTION FI(E1, E2, INTA)

This gives the value

$$\int_{E_1}^{E_2} (E-E1)*F(E)dE \qquad \text{if INTA=1}$$

$$\int_{E_1}^{E_2} F(E)*\log(E/E1)dE \qquad \text{if INTA=2}$$

These segments are to be programmed by the user when an analytical averaging spectrum is chosen.

2./ Spectrum given by point wise /key-number=number of spectrum points/ Energy points should be given in ascending order.

4.3 The card input for NEWZEB and COMMONS for general purpose

The card input of NEWZEB for one task is described in the Table 4.1. The card input is controlled by the leading

segment INZEB.

The COMMONS for general purpose are described in Table 4.2.

Table 4.1 NEWZEB card input

No	FORMAT	I/O list	Multiplicity	Condition	Remarks
1	714	KDAT,NLIB,NGL, NGO,NMAT,NP NPUN	-	-	KDAT=0 return to the MAIN
2	I10	LA			
3	I4	NI		NGO=-1	
4	2E12.5, 214	EP,EM,MK,JI	NI	NGO=-1	
5	6E12.5	EG(I),I=1, NGO+1	NGO/6+1	NGO>0	
7	I10,I4	MATN,NTYP			for each material
8	5(I10,I4)	NTNAM,NFEL	(NTYP-1)/5+1		
9	614	NR1,NR2,NT1, NT2,NSI1, NSI2	NTYP		
10	214	NPAR1,NPAR2			
11	6E12.5	PAR1(I), I=1, NPAR1	(NPAR1-1)/6+1	NPAR1>0	
12	6E12.5	PAR2(I), I=1, NPAR2	(NPAR2-1)/6+1	NPAR2>0	
13	I4,E12.5	NUJM,ERR			

Table 4.1 /cont./

Explanation

KDAT - the task number
NLIB - logical number of RFOD
NGL - logical number of binary SFGK
NGO - key-number for group system
NMAT - number of materials
NP - key number for averaging spectrum
NPUN - logical number of the formatted SFGK

LA
- = 1 open a new binary SFGK
- > 0 binary SFGK is continued from the LA-th word
- =-1 binary SFGK is continued from its end

NI - number of coarse groups
EP,EM - upper and lower boundaries of a given coarse group
MK - number of fine groups in a given coarse group
JI =
- 1 coarse group is divided linearly
- -1 coarse group is divided logarithmically

NTYP - number of group constant types to be calculated
NTNAM - name of the group constant type
NFEL - the serial number of the block to be used
NR1,NR2 - first and last group in the calculation
NT1,NT2,NSI1,NSI2 - first and last parameters from the series or the first and second parameters, respectively
NPAR1,NPAR2 - number of first and second parameters
PAR1 (...), PAR2 (...) values of the first and second parameters, respectively
NUJM - $2^{NUJM}+1$ - the maximal number of points taken in the Romberg integration procedure /NUJM $\leq$ 20/
ERR - required accuracy in the Romberg integration

Table 4.2 COMMONS for general purpose

NAME	LENGTH	
ABSC	5	LC1,LC2 - AA of the last word of the ToC and DH-s, respectively LA - AA on the binary SFGK NT,NSI - number of first and last parameters, respectively
LCLCLC	5	LC,NS1,NS2,NSK1,NSK2
IDENT	7	MATN,NTNAM,NFEL,KDAT,NR1,NR2,NL
PEIF	5	NIN,NOUT - logical number of card input and printer, respectively NLIB,NGL,NPUN
DOPT	3	NG - number of group NP - key number for averaging spectrum AM - mass limit for Greuling-Goertzel approximation
ACCU	2	NUJM,ERR

For the variables LC,NIN,NOUT, and AM value should be assigned either in the MAIN or by BLOCK DATA.

4.4 Output of the NEWZEB

There are three possible outputs of the results of a NEWZEB run:

1./ Binary output /unformatted SFGK/
2./ Card image BCD output /formatted SFGK/
3./ Outprint with commentary

The structure of an unformatted SFGK data set is given in Table 4.3a. The address of a data set is the AA of the word with 'BEGIN'. After the last set of an SFGK file the word with 'END' is written. By continuing the SFGK file the 'BEGIN' of the new set overwrites the 'END'.

Information on the formatted SFGK is given in Table 4.3b

The output is controlled by the segment
SUBROUTINE VIVOD (ID,GC,BF,NGL,NOUT,NPUN)
where

NGL,NOUT,NPUN are logical numbers of peripheries for unformatted SFGK, Outprint and formatted SFGK, respectively. Output with zero logical number is omitted
GC (...) are the calculated group constants /further: real part of SFGK/

At the beginning of VIVOD a segment

SUBROUTINE VIFORM (GC,ID,BF)

is called. In the normal case this is a dummy segment and can be freely programmed by the user if a subsequent transformation of the calculated group constant is needed /e.g. normalization, total inelastic cross-section from UK data etc./

The outprint of the results is self-explanatory.

Table 4.3a. Structure of one set on the unformatted SFGK

Word	Content	Type
1	'BEGIN'	Hollerith
2	MATN	integer
3	NTNAM	
4	NFEL	
5	KDAT	
6	NR1	
7	NR2	
8	NL	
9÷NL+8	GC(...)	real

Table 4.3b. Structure of one set on the formatted SFGK

Card	Format	Content
1	6I12	MATN,MTNAM,NFEL,KDAT,NR1,NR2
2	I12	NL
3 and so on	6E12.5	GC(...)

4.5 Blocks for group constant calculation

4.5.1 General form of the main subroutine of a block

The main segment of a block has the form
SUBROUTINE BLOn (<N_{DH}>, <PAR>, EG,ER,FL,BFG,BFK,WORK,LFR)
where
<N_{DH}> → $N1_{DH}$(...), $N2_{DH}$(...) are the data headings of the nuclear data to be used.

PAR → PAR_1, PAR2,... are non-standard parameters. They can be either vectors or scalars.

BFG(...) - buffer for the RFOD to be used
BFG(...) - buffer for the unformatted SFGK

Further the existing 10 blocks will be discussed. For each block the following information is to be given:

1. Name and the definition of the group constants to be calculated
2. Required nuclear data types
3. Required non-standard parameters
4. The quantities in the real part of SFGK
5. Required length of the dynamic field
6. Action in the case of absence of any required data

When an overlay structure for NEWZEB is used, it is recommended that the different blocks and their auxiliary routines be placed in different overly segments.

If required, each block can be used independently from the organizing part. In this case a main program should be written in order to assign values to the formal parameters and the COMMON variables.

4.5.2 Description of the blocks

Block 1. calculates the infinite dilute spectrum averaged cross-sections <σ_x> /formula /3.1.1// from point-

-wise given nuclear data, any other average $\langle f(\sigma_x)\rangle$ may also be calculated. The function f(x) should be given by the segment

FUNCTION FIQ(X)

In the standard case FIQ=1/X^n if n≠0 and FIQ=X if n=0, and the name of the group constant is 10000xn+NTN. The value n will be included in COMMON/INTG/IN.

Non-standard parameters are not required.

The real part of SFGK contains the calculated group constants from the group NR1 to NR2.

The required length of the dynamic field is

$$L_{block_1} = NR2-NR1+4+(NDAT)_{NR1,NR2} + MAX(NDAT_i)$$

where

$(NDAT)_{NR1,NR2}$ = number of energy points of the cross-section covering the interval of groups from NR1 to NR2

$NDAT_i$ = the same for the group i.

If the required cross-section is not found in the RFOD then all constants are 0.
If the lowest energy point of the cross-section is higher than the lowest group boundary then $\sigma_x = 0$ is taken at that boundary. If the upper group boundary is higher than the last energy point of the data set then $\sigma_x = \sigma_x(NDAT)$ is taken at that boundary.

Block 2. calculates the Greuling-Goertzel constants from the angular distribution of the elastic scattered neutrons /see 3.6.3/. The type name is arbitrary. The required data types are the angular distribution of the elastic scattered neutrons given by pointwise or by Legendre expansion coefficients and the atomic mass A.
A is a non-standard formal parameter.

If A ≤ AM then the parameters μ, ξ, ξ^*, Γ, M and Z /NGRUL=1/, otherwise only μ and ξ /NGRUL=0/ are calculated.

The real part of the SFGK is

$$(\mu_i,\ i=NR1,NR2),\quad (\xi_i,\ i=NR1,NR2)[\xi_i^*,\ i=NR1,NR2),$$

$$(\Gamma_i,\ i=NR1,NR2),\quad (H_i,\ i=NR1,NR2),\ (Z_i,\ i=NR1,NR2)],A$$

The quantities in [...] are given if A≤AM
The length of the required dynamical fields is

$$L_{block_i} = (NR2-NR1+1)*(2+4*NGRUL)+(MANG+6)*IZ_{max}+2*NDAT_{max}+1$$

where

MANG - is the number of angle points used in the integration. In the recent version MANG=21

IZ_{max} - maximal number of angular distribution covering a group

$NDAT_{max}$ - is the maximal number of angle points or maximal number of Legendre expansion coefficients given on the evaluated file.

If no angular distribution is given in the evaluated data file then the angular distribution is taken to be isotropic everywhere and the Goertzel-Greuling constant are calculated by formulae /3.6.3/

Block 3. calculates the inelastic transfer matrix in the fast region. The name of the group constants is arbitrary. If the last excitation level belongs to the unresolved region /continuum/, then only the inelastic excitation level cross-sections /NTN=1005/ are required, otherwise the total inelastic cross-section /NTN=1004/ is also needed. The atomic mass A is the only required non-standard parameter.

The real part of the SFGK is the following:

$$(<\sigma_{in}>^i, i=NR1,IGS),((\sigma_{in}^{i\to j},\ j=1,\ NGO),\ i=NR1,IGS),\ RIGO$$

where

IGS=MINO(IGO,NR2), RIGO=IGO+0.01

IGO - is the group containing the threshold energy of the first excitation level.

Thus the length of the real part of SFGK is

$$NL=(IGS-NR1+1)*(1+\frac{2*NGO-NR1-IGS+2}{2})+1$$

The required length of the dynamical field is

$$L_{block} = NL+NDAT_{max}+MAX(2*MAX(NDAT_j^k),3*MAX(NDAT_j^{tot}))$$

where

$NDAT_{max}$ - is the number of energy points in the largest set of inelastic excitation level cross-sections

$NDAT_j^k$ - the number of energy points of the k-th level cross-section in the group j.

$NDAT_j^{tot}$ - is the number of energy points of the total or unresolved inelastic cross--section in the group j.

If no level excitation cross-sections are given then the total /or unresolved/ inelastic cross-section and the evaporation model are used for the inelastic transfer matrix calculation.

If all inelastic information is missing then all constants are zero.

It is assumed that the values of the inelastic level excitation cross-sections in the first two energy points are zero.

Block 4, block 6, and block 7. calculate the infinite diluted and resonance screened group averaged cross-sections /see 3.3/ from

- pointwise given cross-sections /block 4/, required data types: 1001, 1002, 1102, 1018
- resolved resonance parameters /block 6/, required data types: 5152, 458, 459

- unresolved /statistical/ resonance parameters /block 7/,
  required data types: 5153, 5155 458, 459

The name of group constants is arbitrary.
The temperatures T(...) and the σ_o(...) are specified by input and are given over as non-standard parameters
A, $\lambda\sqrt{E}$, R are non-standard parameters for blocks 6 and 7
IS - spin in the ground state, EB - the binding energy of the last neutrons are further non-standard parameters for the block 7.

The results in the SFGK are stored in the form

RNT,RNSI, $(\langle\sigma_t\rangle_\infty^i$, i=NR1,NR2), $(\langle\sigma_\gamma\rangle_\infty^i$, e=NR1,NR2), $(\langle\sigma_s\rangle_\infty^i$ i=NR1,NR2), $(\langle\sigma_f\rangle_\infty^i$, i=NR1,NR2), $(\langle\gamma\rangle^i$, i=NR1,NR2), $(((\langle\sigma_t^i(\sigma_o^j, T^k)\rangle^i, \langle\sigma_\gamma(\sigma_o^j, T^k)\rangle^i, \langle\sigma_s(\sigma_o^j, T^k)\rangle^i, \langle\sigma_f(\sigma_o^j, T^k)\rangle^i,$ k=1,NT), j=1, NSI), i=NR1,NR2)

where

RNT=NT+0.01, RNSI=NSI+0.01
NT=NT2-NT1+1, number of temperature values
/for the block 4 NT=1/
NSI=NSI2-NSI1+1 - number of σ_o values.

The length of the results is

NL=2+NT+NSI+(5+4*NSI*NT)*NG

The required length in the dynamic field and the action in the case of absence of data differ for blocks 4,6 and 7

Block 4:

$$L_{block_4} = NL+2*NDAT_{1001\ NR1,NR2} + NDAT_{max\ NR1,NR2} + (NSI+1)*NG + MAX\ (NDAT_{1001})_i + MAX\ (NDAT_{max})_i$$

If NTN=1001 is absent than all constants are 0. In the absence of any other type the corresponding constants are zero.

Block 6:

$$L_{block_6} = NL+13*NDAT_{res}+3*MAX(NDAT_i)+NSI*(36+4*NT+6*NUJM)$$

where

$NDAT_{res}$ - number of resonance parameter sets

$NDAT_i$ - number of resonances in the group i

If no resonance parameters are given in the interval NR1,NR2 then all constants are zero

Block 7:

$$L_{block_7} = NL+8*NDAT_{5153}+22*NSER+4*NSI*NT+2*NSI$$

where

NSER - number of resonance series

If no 5153 then $\bar{D}=1$, $\nu_n = 1$
If no 5155 then $\bar{\Gamma}_f = 0$
If no 5153 and 5155 then all constants are zero.

Block 5: Calculates the group averaged values of the product of two pointwise given quantities /e.g. $\nu\sigma_f$ or $\mu\sigma_s$. The name of the group constant is 10000xNTN1+NTN2 where NTN1 and NTN2 are the type names of the first and second quantities, respectively. Non-standard parameters and data types except NTN1 and NTN2 are not required.

The real part of the SFGK is similar to that of block 1.
The required length of the dynamic field is

$$L_{block_5} = NR2-NR1+1+2*(NDAT_{fi})_{NR1,NR2} + (NDAT_{se})_{NR1,NR2} + 3*MAX(NDAT_{se})_i + MAX(NDAT_{fi})$$

The index fi refers to the first, se to the second data type /according to their occurrence in the evaluated file/,

If any of two types is absent then all constants are zero.

Block 8: calculates the integrals

$$\bar{Q}_{ji} = \int_{E_{i+1}}^{E_i} dEQ(E,par_j)F(E)$$

$$\bar{F}_i = \int_{E_{i+1}}^{E_i} dE\ F(E)$$

by means of the Romberg's procedure where Q(E,par) is a smooth function determined by the series of parameters par. The name of the group constants is 10000xNTN_{10}+NTN_{20}, where NTN_{10} and NTN_{20} are the name of a data types with NTF=10 /or 0/ and NTF=20 /or 0/, respectively. These are the required data types.

There are three methods for specifying the parameters:

1. Data from the type NTN_{10} are taken as parameters
2. Values in the first input parameter field PAR1(...) are taken as parameters,
3. Parameters are given by certain sets of data type NTN_{20}.

The required sets are separated by the parameters given in the second input parameter field PAR2(...). It is assumed that the sets of type NTN_{20} are in ascending order by its first variable, /this is, ordinarily, the energy/ and the values in PAR2(...) are of the same physical meaning. The other variables of the data sets are regarded as a function of this first one and are interpolated linearly to the values given in PAR2(...).

If no data type with NTN_{10} is on RFOD, then no parameters specified by method 1 are expected.

If NT=0 /number of parameters in PAR1(...)/, then no parameters specified by method 2 are expected.

If no data type with NTN_{20} is on the RFOD, then no parameter specified by method 3 are expected.

The real part of SFGK is

$$((Q_{ji},\ i=NR1,NR2),\ j=1,\ NSI),\ (F_i\ i=NR1,NR2)$$

Its length is

$$NL = (NSI+1)*(NR2-NR1-1)$$

The required length in the dynamic field

$$L_{block_8} = NL+N_{par}$$

N_{par} is the number of parameters used in the whole calculation
The function Q(E,par) is generated by

FUNCTION PARFI (E,AP,LP)

LP - number of parameters

AP(...) field containing the parameters.

Block 9: calculates the elastic scattering matrix up to P_5 approximation. In addition to the angular distribution of elasticaly scattered neutrons, the cross-section and the average cosine of elastic scattering are used. The latter is required for the correction of angular distribution (see [8]). if it is absent on the RFOD then no correction is parformed. The name of the calculated group constant is arbitrary. The required non-standard parameter: A - atomic mass.

The real part of the SFGK is

$$NLA+0.01,NLE+0.01,\ (IMAX_i+0.01,\ ((<\sigma_s^{\ell}>^{i\to i+k-1},\ell=1,\ NM1),$$

$$k=1,\ IMAX_i),\ i=1,\ NG)$$

where

$$NG = NR2-NR1+1$$

NLA,NLE - the lowest and the highest Legendre momentum to be calculated

$IMAX_i$ - maximal group change by a scattering in the group i NM1=NLE-NLA+1

The length of the real part of SFGK is

$$NL=2+NG+NM1*\sum_{i=1}^{NG} IMAX_i$$

The required length in the dynamical field is

$$L_{block_9}=35+NL+NM1*IMAX*3+NUJM+MANG*2+NZ+NZ+IMAX+2*NJM+3*NDAT$$

where

$IMAX=MAX(IMAX_i)$

NUJM and NJM are the n_{max} of the Romberg's procedure for energy and angle integration respectively. According to our experience NJM=6 is an optimal value.

NZ - the number of angular distribution covering the groups from NR1 to NR2

If the elastic scattering cross-section is absent from the RFOD then all constants are zero.

If the angular distributions are absent from the RFOD then isotropic angular distribution is taken.

Block 10: calculates the inelastic scattering matrix by the formula (3.5.2). The arbitrary averaging functions, $\chi(E)$ and M(E), may be specified either by the parameters given in the field PAR1(...) and PAR2(...), respectively, /They are the non-standard parameters and there is a restriction: NPAR1+ +NPAR2 $\leq$ 10/, or may be given pointwise. The first/second series of parameters or the first/second spectrum points specify the functions M(E)/ $\chi(E)$. When both spectra are analically given then both should be included in PHI(E). The choice between them is facilitated by the variable NPA which is given over by

COMMON/PARH/PAR (10), NPA

If NPA=1 then M(E)and If NPA=2 then $\chi(E)$ is calculated.
The name of the calculated group constants is arbitrary.
Except the matrix $\sigma_\ell(E_1 \to E_2)$ /NTN=300, NTF=5/ no data type is required.
The length and the content of the SFGK are

NL=2+(NR2-NR1+1)*NGO*NF
NGO+0.01,NF+0.01, $(((\bar{\sigma}_\ell^{i\to j}$, j=1, NGO), i=NR1,NR2), ℓ=1,NF)
The required length in the dynamical field:

$L_{block_{10}}$ = NL+NDAT1+NDAT2+2+NF*NDAT2+NDAT2+NGO*NF*NDAT1$_{NR1,NR2}$

4.6 Diagnostics of the NEWZEB

4.6.1 The check of the length of the required dynamical field

The required length of the dynamical field is checked in some places of the program. When it is insufficient for the further calculation then an error message:

"REQUIRED LENGTH <n> AT DISPOSAL <k>" is given

If this occurs in a block then the calculation is continued with the next group constant type.
If this occurs in the GROP, then the calculation is continued with the next material.
If this occurs in INZEB then a RETURN to the MAIN follows.
The protection from the dynamic field overflow is not perfect. Any abnormal program termination should initially be investigated from this point of view.

4.6.2 Other error messages

The general form of an error message is

ERROR IN <name> NUMBER <n>

where

<name> - name of the segment where the error has taken place
<n> - error type number

If n < 300 then the error is fatal

If n ≥ 300 the calculation is continued /warning/

The error messages are performed by

SUBROUTINE ERROR (NAME,N)

a./ Error in the card input

n

-M no block with number M

201 the group boundaries are not in monotonic descending order

203 the first group to be calculated is below the last one

204 first } parameters to be used are not correctly referred

205 second }

320 the arguments of the averaging function are not in monotonic ascending order

b./ Error in the RFOD

n

301 Negative cross-section

302 arguments of the cross-section are not monotonic ascending

c./ Absence of data

350 the required material is not in the RFOD. The next material is taken

351 the required data type is absent

352 required angular distribution is absent

353 the first required energy point is lower then the lowest data point: cross-section in this point is taken to zero.

354 the last energy point is higher than the highest data point: cross-section is horizontally extrapolated.

5. SERKON - A PROGRAM FOR OPERATION WITH SFGK AND FOR COMPILATION OF GROUP CONSTANT LIBRARIES

SERKON performs the following tasks:

1./ Copy and /or print and/ or punch selected data set from an SFGK file

2./ Compile a group constant library from

a/ constants in an SFGK

b/ constants given by punched card

c/ constants of an older group constant library.

The newly created library can be in binary and /or in BCD card image form.

The name of the leading segment is: SERKON. The input is described in Table 5.1. It should be pointed out that the card of type C can be automatically punched by a trivial program which significantly reduces the manual punching work.

A data set on SFGK is retrieved by

SUBROUTINE ISKDAT (LA,ID, NLIB,BF,NS1, NS2,WORK, LFR)

where

LA $\leq$ the absolute address of the required data set

ID(...) the integer part of SFGK

|NLIB| - logical number of the SFGK file

If NLIB>0 binary SFGK

If NLIB<0 formatted card image SFGK

BF(...) buffer for the SFGK file

NS1,NS2 - buffer position for the binary SFGK file

The compilation of group constant library is performed by

SUBROUTINE GRACLI (ID,GR,LFR,WORK,N)

where

GR(...) are group constants. It is a free subroutine and should be programmed by the user. Recently, a GRACLI for the compilation of the GRACE library [9] has become available.

Table 5.1 Input for SERKON

Card type	Format	Content
A	6I4	N1,N2,NOUT1,NPUN,NGR,NN2 are logical numbers of peripheries for SFGK to be read, for binary SFGK to be written, for lineprinter, for card image SFGK to be written, for binary group constant library and for card image group constant library, respectively
B	I1O	LX - this has the same meaning as LA has in Table 4.1
C	3I12,4I9	LA - data set control number /Table 5.2/ ID(I), I=1,6 integer part of the SFGK set or other control numbers /see Table 5.3/
D	6I12	integer type constants
E	6E12.5	real type constants
F	9A8	Hollerith type constants

Remarks: 1. If N1 $\geq$ 1OOO RETURN to the MAIN
2. Output omitted if the corresponding logical number is zero
3. Card of type B is required only then when N2>O.

Table 5.2 Description of the data set control number LA

LA	Control effect
>0	read from SFGK; next card is of type C
=0	next card is of typa A
-1	next card is of type D
-2	next card is of type E
-3	next card is of type F
-5	all group constants are zero
-10	constants will be taken from an older group constant library

Table 5.3 The meaning of ID(I)

I/LA	>0	0	-1	-2	-3	-5	-10
1	MATN	X	X	X	X	X	X
2	NTNAM	X	NTNAM	NTNAM	NTNAM	NTNAM	N
3	NFEL	X	NFEL	NFEL	NFEL	NFEL	L
4	KDAT	X	NL	NL	NL	NL	NL
5	NR1	X	NR1	NR1	NR1	NR1	K
6	NR2	X	NR2	NR2	NR2	NR2	X

Explanation

X - arbitrary information

N - logical number of the old group constant library

L { < 0 REWIND before READ
  { = 0 no REWIND
  { > 0 REWIND after READ

K { ≥ 0 skip K records forward
  { ≤ 0 skip |K| records backward

before READ

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APPENDIX 1.

Free segments and their standard form

The work of the FEDGROUP system may be controlled by the adequate choice of the following free segments.

PRAFO

SUBROUTINE ERTAPE (N)

This is for the recovery of the errors on the evaluated files, each card of which appears in

COMMON/CROS/SJ (14)
It is activated together with ARED.
Standard form: dummy routine.
Segments, assignig interpolation numbers are
SUBROUTINE INTR (NT,NFT,INTA,INTF)
SUBROUTINE INTW (NT,NFT,IWORK,NW,L3)
SUBROUTINE INTT (NT,INTA,INTF)

In their standard form 1 is assigned to all interpolation numbers except that controlling the interpolation of angular distribution in energy /This is equal to 2/

NEWZEB

SUBROUTINE VIFORM (A,ID,BF)

This is described in 4.4. Its standard form is a dummy routine.

FUNCTION FIQ (A)

Any cross-section value of a pointwise given cross-section which is integrated by means of FXINT /block 1,2,3, 4,5,10/ goes through this function, i.e. σ_x is transformed into FIQ (σ_x). Its standard form

$$FIQ = \begin{cases} A \text{ if } N=0 \\ (1/A)^N \text{ if } N > 0 \end{cases}$$

where N is given over by

COMMON/INTG/N

and specified by input /see 4.5.2 block 1./

FUNCTION PHI(E)

gives the spectrum value F(E). The standard spectrum is

$$F(E) = \begin{cases} 1/E \text{ if } E \leq 1.4 \times 10^6 \text{ eV} \\ Ce^{-E_m/0.965}\left(e^{\sqrt{2.29\ E_m}} - e^{-\sqrt{2.29\ E_m}}\right)/2 \end{cases}$$

and a proper choice of C ensures the continuities of F(E)

FUNCTION PSI (E1,E2)

gives the value of $\int_{E_1}^{E_2} F(E)dE$.

FUNCTION FI (E1,E2,INTA)

gives the value

$$\int_{E1}^{E2} \begin{cases} \log(E/E1) & \text{if INTA=2} \\ (E-E1) & \text{if INTA=1} \end{cases} F(E)dE$$

The forms of FI and PSI are generally fitted to that of PHI.

FUNCTION PARFI (E,AP,L)

gives Q(E,par), for the integration in the block 8. Its standard form is a Crainberg spectrum

$$Q(E,A,B,C) = 0.5 \times A \times e^{-\sqrt{BE}}\left(e^{\sqrt{CE}} - e^{-\sqrt{CE}}\right)$$

where the parameters are A=AP(1), B=AP(2), C=AP(3).

SERKON

SUBROUTINE GRACLI (ID,WORK,LFR,GR,N)

This compiles the required group constants library. Its standard form compiles the GRACE library.

In the standard source deck of FEDGROUP the standard forms of the free segments are given.

APPENDIX 2.

a, Generation of cross-sections for a given set of energy points from pointwise given cross-section

This is an application offered by the free subroutines. The followings should be taken.

```
      SUBROUTINE VIFORM (A,ID,BF)
      DIMENSION  A(1),  ID(1), BF(1)
      COMMON/DOPT/NG,NP,AM
      COMMON/SPOINT/S(120),NL
      IF(ID(3). NE.0)GOTO 1
      IF(ID(2). EQ.2)RETURN
```

Here the group boundaries should be assigned to the elements of the field A. and the lower group boundaries to the elements of the field S , respectively. NL and NG are the number groups.

```
1     CONTINUE
      RETURN
      END
      FUNCTION PSI (E1,E2)
      COMMON/SPOINT/A(120), NL
      PSI=0.
      DO 1 I=1, NL
      IF(E1.EQ. A(I))GOTO 2
1     CONTINUE
      RETURN
2     PSI=1.
      RETURN
      END
      FUNCTION FI (E1,E2,INTA)
      FI=0.
      RETURN
      END
```

We have the pointwise cross-sections in the place of group constants by using block 1.

b, Pointwise cross-sections from resonance parameters

The SUBROUTINE VIFORM in this case is almost the same as in the previous one. The difference is that points for the cross-sections are identical with the lower boundary of every second group. The FI and PSI are of no concern but for the spectrum function we have

```
      FUNCTION PHI(E)
      COMMON/SPOINT/S(10), NL
      PHI=0.
      D O 1 I=1, NL
      IF(S(I)NE,E) GOTO 1
      PHI=1.
      GOTO 2
1     CONTINUE
2     CONTINUE
      RETURN
      END
```

We get the pointwise cross-sections in place of group constants by using block 6 or 7 twice for every point.

APPENDIX 3.

Resonance integrals for Pu239 calculated from different files

In the report [*] /page 20/ resonance integrals for Pu239 are given. In the Table the corresponding values calculated from the data of the files KEDAK, UKNDL /DFN=404/, SOKRATOR /evaluated by V.V.Konshin/ and LENDL /DFN=7176/ are demonstrated.

[*] M.F. Vlasov et. al. INDC/NDS/-47/L

The resonance integrals of Pu239 calculated from the data of different evaluated files ($I_x = \int \sigma_x \frac{dE}{E}$)

		KEDAK	UKNDL	SOKRATOR	LENDL	Reported in [x]
0.5-4.65eV	I_f	83.8	80.1	64.9	87.7	
	I_γ	31.9	25.8	25.4	33.0	
4.65eV-10keV	I_f	205.8	212.3	201.0	205.5	202.1
	I_γ	173.5	175.4	144.0	166.0	147.6
10keV - 1MeV	I_f	7.56	7.27	8.56	7.55	
	I_γ	1.48	1.64	1.62	1.47	
0.5eV-1MeV	I_f	297.2	299.7	274.5	300.8	300.0±10
	I_γ	206.9	202.8	171.0	200.5	181.±15

APPENDIX 4.

Names of certain subroutines on the standard FEDGROUP source deck

As has been mentioned there are subroutines which depend on the structure of the original evaluated file. This means that on the FEDGROUP source deck there should be different subroutines with the same name.

In order to avoid this inconvenience different names are assigned to these subroutines /but the call is performed with the original name/. The original names and the related subroutines are shown in the next Table.

Name in CALL	OK,KEDAK file	ENDF/B	SOKRATOR		ENDL
			U238	PU239	
ARED	ARED	ARED	ARED8	ARED	ARED
SARED	SARED	-	SARED8	SARED	-
ARED1	-	-	ARED18	ARED1	-
SOKSLV	-	-	SOKSL8	SOKSLV	-
SOKEL	-	-	SOKEL8	SOKEL	-
FINDEL	FINDEL	FINDFB	-	-	-
ERTAPE	ERTAPE	-	ERTAPE	ERTP9	ERTAPE
SKIP	SKIP	SKIPE	-	-	-

APPENDIX 5.

Test cases for FEDGROUP /ISPRA CPL version/

1. Generation of RFOD for U238 /file UKNDL, DFN=160/ and calculation of group averaged infinite dilute cross--sections /BLOCK 1/ and inelastic transfer matrix /BLOCK 3/ for the group system ABBN.

2. Calculation of Greuling-Geortzel constants for O-16 /KEDAK file/ for 40-group GRACE system /BLOCK 2/

3. Generation of RFOD for Fe /file KEDAK/ and calculation of screened group-averaged cross-sections

4. Calculation of $\nu\sigma_f$ for the U235 /file UKNDL, DFN=271/ for the group system ABBN

5. Calculation of screened group-averaged cross-sections from resolved resonance parameters for U235. Group system: ABBN. Resonance parameters are taken from the file KEDAK /BLOCK 6/

6. Calculation of screened group averaged cross-sections from unresolved resonance parameters of the U235. Group system: ABBN. Resonance parameters are taken from the file KEDAK /BLOCK 7/

7. Calculation of group fission spectrum from Watt formula. Parameters are given by input. Group system ABBN /BLOCK 8/

8. Calculation of elastic transfer probabilities in P_1 approximation for oxigen /BLOCK 9/

NOTATIONS AND ABBREVIATIONS