International Atomic Energy Agency

INDC(HUN)-15/L

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

FEDGROUP - A PROGRAM SYSTEM FOR PRODUCING GROUP CONSTANTS FROM EVALUATED NUCLEAR DATA OF FILES DISSEMINATED BY IAEA

P. VÉRTES

Central Research Institute for Physics
P.O.B. 49, H-1525 Budapest, Hungary

(Revised version of INDC(HUN)-13/L)

March 1978

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

Reproduced by the IAEA in Austria
March 1978
78-2056

FEDGROUP - A PROGRAM SYSTEM FOR PRODUCING GROUP CONSTANTS FROM EVALUATED NUCLEAR DATA OF FILES DISSEMINATED BY IAEA

P. VÉRTES

Central Research Institute for Physics
P.O.B. 49, H-1525 Budapest, Hungary

(Revised version of INDC(HUN)-13/L)

March 1978

1. INTRODUCTION

The program system FEDGROUP was originally released for general distribution in June 1976. At present, it is used in four CMEA countries: Hungary, USSR, Poland and GDR. It is widely applied for the generation of group constant libraries used by different spectral codes. During its use a number of errors were detected and a number of other deficiencies in the performance of the program have been eliminated. Misprints and omissions in the basic report INDC/HUN/-13 have also been found.

In this revised version, released in November 1977, the programming errors have been removed and an extension is introduced. This extension is described in section 2.

The basic computer of FEDGROUP is the CDC-3300. There exist, however, CYBER-72, BESM-6 and IBM-360 versions, too. The problems connected with the various computer versions are discussed in section 3.

In section 5 results of test calculations are quoted.

Finally, the errata to the report INDC/HUN/-13 are given.

2. CALCULATION OF THE GROUP AVERAGED FLUX AND GROUP CONSTANTS FOR BIOLOGICAL SHIELDING

In some cases it is also useful to have the group averaged flux, i.e.

$$\int_{E_{i+1}}^{E_i} \varphi(E)dE = \varphi_i$$

By means of φ_i two adjacent groups can be merged, i.e. group constants can be calculated by

$$\sigma_{i+(i+1)} = \frac{\sigma_i\varphi_i + \sigma_{i+1}\varphi_{i+1}}{\varphi_i + \varphi_{i+1}}$$

The group averaged flux can be used for the calculation of group diffusion constants too. The second P_1 equation is

$$1/3\nabla\phi^1 + \Sigma^i J^i = \sum_{\vec{\gamma}} \Sigma_1^{j\to i} J^j$$

The diffusion approximation may be derived by the assumption of Fick's law:

$$J^i = -D^i * \mathrm{grad}\varphi_i$$

where D^i is the diffusion constant.

If in a given part of reactor or shielding

$$\phi_i = \varphi_i \Psi(r)$$

is assumed then we have

$$D^1 = \frac{1/3 + \sum_{j\neq i} \Sigma_1^{j\to i}\varphi_j/\varphi_i}{\Sigma_{tr}^i}$$

where

$$\Sigma_{tr}^i = \Sigma_t^i - \Sigma_1^{i\to i}$$

This means that D^i can be calculated from σ_t^i, φ_i /BL01/ and from $\sigma_1^{j\to i}$ /BL09/. Using $\sigma_o^{i\to i}$ /BL09/ the removal cross-section can be calculated

$$\sigma_{rem}^+ = \sigma_t - \sigma_o^{i\to i}$$

The calculation of the group averaged flux is introduced in blocks 1,4,6 and 7. The outputs of these blocks are changed as indicated in the following part.

3. FEDGROUP ON COMPUTERS OTHER THAN CDC-3300

FEDGROUP is adapted to CYBER-72, BESM-6 and IBM-360. Deviations are mainly due to the different I/O operations of different computers but some difficulties have arise because of the restrictions imposed on the permitted values of constants.

The compilers CYBER-72 and BESM-6 are similar to that of CDC-3300, the possibilities of CYBER even larger. However, the maximum order of real numbers on BESM-6 is 10^{19} and a number less than 10^{-19} is taken to be zero. This leads to fatal errors in some special cases /e.g. where energy points fall too near to each other/. This has been experienced in the segments

FXINT /interpolation formula/
W from label 13 up to 64: TEMP7 may be too small.

In these cases there can be a ratio of two small numbers. By a slight modification of the segment both of these difficulties can be avoided.

In the case of IBM software, the difficulties are:

1. The lack of ENCODE and DECODE statements. They occur in PRAFO programs very frequently /except LENDL/ and once in SERKON. The application of BUFFER IN and DECODE statements allowed us to read IBM tapes directly /where the evaluated data appear/ and to repeat the reading of a card without BACKSPACE. In the case of IBM software this effect can be achieved by writing some of the cards to a direct access temporary file and thereafter reading them with corresponding format conversion. The reading and writing of the cards to the temporary file are controlled by ARED thus the structure of the program is not changed in the IBM version only

the DECODE's are changed to READ.

2. The lack of BUFFER IN and BUFFER OUT statements. They occur only in the segments ARED, BUFIN, OUTR and in these cased BUFFER IN and BUFFER OUT should be changed to READ and WRITE, respectively.

3. The number of characters in a word is 4 instead of 6 or 8. This causes a slight change in some data statements. The first word of an SFGK data set will be BEGN rather than BEGIN. Fortunately, no literal information is to be stored in the dynamical field except the comment part of RFOD.

4. Because of the shorter word /32 bits instead of 48/ the accuracy may be reduced in some cases. Up to now, it is not known what changes will be brought about by this deviation. The numerical names of elements of UKNDL and ENDF/B files should be shortened.

4. PROCESSING OF LARGE DATA SETS

In the recent version of the KEDAK file there are data sets with more than 9000 energy points. Users working with smaller computers find themselves in difficulties with the dynamical field requirement since for running the KEDAK subroutine over 12000 words are needed.

This problem can be solved by gathering the function values on the RFOD file to be produced rather than to store them in the fast memory. After processing the data set the function values need to be coped from RFOD to the auxiliary file.

5. TEST CALCULATIONS

The test numbers given by us do not represent a whole sample calculation. Sample calculations which would reflect the operation of each part of the system would be extremely cumbersome. Therefore we list a series of test numbers which reflect the system operation but we omit the details of the input data

and of the printed output.

Unless otherwise indicated the ABAGYAN type 26-group system and the standard reactor spectrum built in the program are used. The same series of calculations was repeated with point-wise spectrum. This point-wise spectrum consisted of 100 points which described the standard spectrum. The experienced small deviation of results is good evidence for the correct working of the program system in the case of the point-wise spectrum option.

1. Infinite diluted group avraged constants /Block 1/
   Group system: Abagyan-26
   Averaging spectrum: standard
   Material: U-235 /KEDAK, 1970/

Data type \ group	5	15	20
total 1001	6.71277	28.9204	118.269
fission 1018	1.22256	11.4868	46.3767
absorp. 1102	9.9102E-2	4.35755	58.4140

2. Greuling-Goertzel constants /Block 2/
   Group-system: Abagyan-26
   Averaging spectrum: point-wise
   Material: O-16 /KEDAK 1970/

Quant. \ group	1	8	10
μ	0.212308	2.9410E-2	4.20277E-2
ξ	9.94453E-2	0.122537	0.120943
ξ^*	9.15512E-2	0.122944	0.120953
η	8.11995E-2	8.30452E-2	8.23669E-2
Γ	-4.56092E-2	-3.83487E-2	-3.68556E-2
H	0.132113	0.127731	0.129883

3. Inelastic transfer matrix /Block 3/
   Group system: Abagyan-26
   Averaging spectrum: point-wise
   Material: U-235 /KEDAK 1970(1), UKNDL 271 (2)/

From group i \ to group		i	i+1	i+2
2	(1)	3.98806E-4	1.64073E-2	1.92433E-1
	(2)	3.47060E-4	1.42128E-2	1.66086E-1
10	(1)	1.3238E-2	4.54865E-3	0.0
	(2)	1.14376E-2	7.28607E-3	2.68634E-4

4. Resonance screened group-averaged cross-sections from point-wise given data /Block 4/
   Group system: Abagyan-26
   Spectrum: point-wise
   Material: O-16 /KEDAK 1970/
   Group: 3

Data type \ σ_o	0	10	100	1.0E4	∞
total 1001	1.60657	1.89148	1.94766	1.95533	1.95541
elastic 1002	1.60489	1.88914	1.94523	1.95289	1.95297
flux	4.40632E-1	5.34278E-2	6.14738E-3	6.2536E-5	6.2547E-1

5. Group averaged values of the product of two point-wise given quantities /Block 5/
   Group system: Abagyan-26
   Spectrum: point-wise
   Material: Pu239 /UNKDL 404/

Group	3	15
$\nu\sigma_f$	6.32535	25.7292

6. Resonance screened group averaged cross-sections from resolved parameters /Block 6/

Group system: Abagyan-26

Spectrum:standard

a/ Material: U235 /KEDAK 1970/, single-level (1), multi-level (2)

NUJM=6, T=300 K, group: 18, ERR=0.01

Data type \ σ_o		0	10	100	∞
total	(1)	34.2362	38.0229	49.9399	64.7643
	(2)	34.4809	38.2249	50.0619	64.8047
absorption	(1)	9.76128	11.3922	16.6253	23.1341
	(2)	9.80445	11.4221	16.6369	23.1340
elastic	(1)	11.8034	11.9439	12.3122	12.7370
	(2)	11.9467	12.0744	12.4062	12.8066
fission	(1)	12.6678	14.6922	21.0122	28.9507
	(2)	12.7258	14.7336	21.0300	28.9506
flux	(1)	2.27928E-2	1.61623E-2	5.13016E-3	0.765718
	(2)	2.26331E-2	1.60962E-2	5.12611E-3	0.765718

gamma = 0.945497 (1), 0.945480 (2)

b/ Material: U235 /ENDF/B standard/

Multilevel, NUJM=4, ERR=0.01, T=0.0K, group: 22

Data type \ σ_o	0	100	1.E4	∞
total	30.0683	35.6287	39.5457	39.6351
absorption	3.74261	5.38287	6.79476	6.82805
elastic	13.3120	13.3558	13.3692	13.3695
fission	12.9901	16.8617	19.3840	19.4396
flux	3.70747E-2	6.10524E-3	7.69107E-5	0.771402

gamma = 3.04459E-1

7. Resonance screened group averaged cross-sections from unresolved parameters /Block 7/.
   Group system: ABAGYAN-26
   Spectrum standard
   Material: U235 /KEDAK 1970/
   Group: 14, T = 300 K^{O}

Data type \ σ_o	0	1000	10000	∞
total	20.7661	22.8565	22.9098	22.9100
absorption	2.68582	3.29266	3.30815	3.30830
elastic	12.1312	12.3128	12.3182	12.2771
fission	5.9880	7.2917	7.32456	7.32488
flux	4.28664	4.59713	4.60543	4.60553

8. Integral of an analytical function given by parameters /Block 8/

This block may be tested by any function the integral of which can be easily calculated analytically. Therefore no sample calculation is given.

9. Calculation of elastic scattering matrix /Block 9/
   Group system: Abagyan-26
   Spectrum:standard
   Material: O-16 /KEDAK 1970/

Moment / group	3		12	
	3 → 3	3 → 4	12 → 12	12 → 13
0	0.71351	0.11337	2.3855	0.44764
1	0.24462	-0.25492E-1	0.25466	-0.13652
2	0.15590	0.72134E-6	9.6741E-3	-7.4209E-3

10. Calculation of the inelastic transfer matrix in the thermal region /Block 10/

In lack of outgoing data an artificial test has been created by giving the inelastic point-wise transfer matrix in the form

$$\sigma_n(X \to y) = f_n(x) g_n(y)$$

where

$$f_n(x) = x^{n+1}$$

$$g_n(y) = \frac{1}{1+y^{n+1}}$$

$n = 0 \div 2$, and the interval of the energy variables are $0 < x < 10$ and $0 < y < 11$. The energy points are determined

$$x_i = (i-1)\frac{10}{(N_x-1)} \text{ and } y_j = (j-1)\frac{11}{(N_y-1)}, \text{ respectively,}$$

where $N_x = 30$, $N_y = 40$

The spectra are determined by

$$M(E,T_1) = \begin{cases} E^* e^{-E/T_1} & \text{if } E \leq 1.1 \\ 1.21^* \dfrac{e^{-1.1/T_1}}{E} & \text{if } E > 1.1 \end{cases}$$

and

$$\chi(E,T_2) = M(E,T_2) + E^*Q$$

where T_1, T_2 and Q are parameters to be specified on cards 11 and 12, respectively, of NEWZEB input.

Sample numbers from the results /the group boundaries are given in parenthesis/:

from to	MOMENTUM		
	0	1	2
(10.,6.31)→(2.,0.)	7.3067	65.299	564.63
(0.4,0.2) →(2.51,1.58)	0.10207	2.2262E-2	4.8399E-3
(1.,0.8) →(0.8,0.6)	0.53147	0.56198	0.58989

The point-wise spectrum used in the calculations is defined by

$$x_i = \begin{cases} 0.1*i & \text{if } i \leq 10 \\ 1.E7*e^{-(100-i)*\Delta u} & \text{if } i > 10 \end{cases}$$

where $\Delta u = 7*\log 10/89$

Errate and adenda to the report INDC/HUN/-13

In the case of text an erratum is defined by n/m<X>/<Y>, where

n - number of page

m - number of row

<X> { = T from the top
B from the bottom

<Y> { = A add the following row/s/
Rk replace k subsequent row/s/ by the following row/s/
Dk delete k subsequent row/s/.

In the case of a Table an erratum is defined by $n(n_p)/m,k/<Y>$, where

n - number of the Table on the page n_p

m - number of entry /for the heading m=0/ on the page n_p

k - number of column; if k=0 then the correction relates to the whole entry

Y { = A add the following entry
R replace the column in the entry
Dk delete the k subsequent entry

A formula is taken for one row.

5/15T/A

$i_7 i_6 i_5$ - atomic number of isotope

2.1(10)/7,2/R

2+NW+MFN*(NW+5)

2.1(10)/3,4/R

ARG1(NDAT1), ARG2(NDAT2), FUN(NF, NDAT2, NDAT1)

9/5T/A

By this time only the lin-lin and log-lin interplation schemes are taken into account in the calculations.

2.2(13)/2,3/R

$t\sqrt{E}$ - reduced wavelength: R - nuclear radius; E_b - binding energy of the last neutron

2.2(13)/3,3/R

average level density: a and $2\sigma^2$ are constants for statistical theory

2.2(14)/2,0/A

3019|4| neutron incident energy; A,B,C are parameters for the Crainberg fission spectrum

2.2(14)/5,0/A

3018	neutron incident energy	neutron outgoing energy	prompt fission spectrum

17/4B/A

NAME - name of the material on the original file

2.4(18)/4,3/R

KU = | 0 UK file
| 1 for KEDAK*

2.5a(19)/3,9/R

20

2.7(22)/5,3/R

NTN,NF,NS are type names on the RFOD, file and section number on the outgoing file, respectively

26/8T/R

In the first case let $\sigma(E)$ be given at point E_j,

30/1T/R

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

30/3T/A

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

30/5B/R

g - statistic spin factor

Taking $\alpha_r \equiv \beta_r \equiv 0$ in /3.2.1/ we return to the single level formula

31/10T/R

$$D = D^o\left(\frac{EB+E}{EB}\right)^{1.25}\exp(-89.72\sqrt{EB+E} + \sqrt{89.72EB})$$

31/4T/R

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

31/1B/A

The difference in the results of the last two steps of Romberg's procedure gives the uncertainties of the integration in the given interval. They are summed up and the sums are divided by the group flux. So we get the absolute uncertainty of the group averaged cross-sections. These uncertainties are printed out when there is no convergence.

36/7B/R

SUBROUTINE RESCAL (EP,FM,NA.JR,RPAR,SGT,SGS,SGI,SGF,WORK,

42/13B/A

The results - deviating from MIGROS-2 - will not be divided by $\Sigma_j \sigma_o^{i\to j}$

46/8B/R2

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

4.1(51)/5,0/A

6|6E12.5|ER(I),FL(I),I=1,NP|(NP-1)/3+1|NP>1

51/1B/A

Note: if in block 6 the single level Breit-Wigner formula is required then ERR should be given with negative sign.

56/11T/R

BFK(...) - buffer for the unformatted SFGK

50/4B/A

3./ Spectrum given step-wise /key-number=number of steps+1/. Last energy point should be >1. E9 in order to recognize this case.

57/10T/R

Constants from the group NR1 to NR2 and the group averaged flux from the group NR1 to NR2

$$NL=2*(NR2-NR1+1)$$

57/12T/R

$$L_{block_i}=NL+3+(NDAT)_{NR1,NR2}+MAX(NDAT_i)$$

58/1B/R

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

60/11T/R4

$$RNT,RNSI,(T_i,i=1,NT),(\sigma_{o_i},i=1,NSI),(<\sigma_t>_\infty^i,i=NR1,NR2),$$
$$(<\sigma_\gamma>_\infty^i,i=NR1,NR2),(<\sigma>_{s\infty}^i,i=NR1,NR2),(<\sigma_f>_\infty^i,i=NR1,NR2,(<\gamma>)^i,i=NR1,NR2),$$
$$(((<\sigma_t(\sigma_o^j,T^k)>^i,\ <\sigma_\gamma(\sigma_o^j,T^k)>^i,\ <\sigma_s(\sigma_o^j,T^k)>^i,\ <\sigma_f(\sigma_o^j,T^k)>^i\ k=1,NT),$$
$$j=1,NSI),\ i=NR1,NR2\ ,(((\phi_{kj}^1,\ k=1,NT,),j=1,NSI),\ i=NR1,NR2),(\phi_i^\infty\ i=NR1,NR2)$$

60/8B/R

NL=2+NT+NSI+(5+4*NSI*NT)*NG+NG*(NSI*NT+1)

61/6B/R

Block 1, except that no fluxes are given.

63/13T/A

The parameters in field AP are placed in the respective order in which they arrive from NTN_{10}, PAR1(...) and NTN_{20}.

65/1T/A

The point-wise spectra should be given on the input cards of type 6. The spectrum M(E) should be the first. It is assumed that only the lowest energy point of $\chi(E)$ is lower than the highest energy point of M(E).

5.1(68)/2,3/R

LX - which has the same meaning as LA in Table 4.1. This card is required only if N2 ≠ 0

5.2(69)/3,2/R

next card is of type E

5.2(69)/4,2/R

next card is of type D

74/5T/R

The following example shows how to do this.

81/9B/R

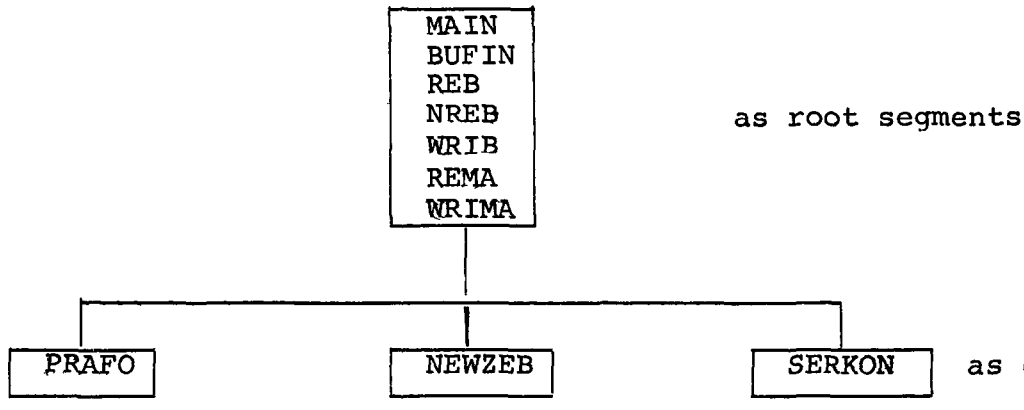
ID(...)	68	NPAR1,NPAR2	53

81/18T/R

FEDGROUP	1	NFEL	52

Overlay suggestions

a./ Overlay for the whole FEDGROUP system



Note: PRAFO's for different evaluated files may be parallel in OVERLAY B. In this case their common routines such as, e.g. ARED, SLOV are in OVERLAY A.

b./ The NEWZEB is a large program therefore it has it own overlay structure, as shown on the next page.

Overlay for NEWZEB