OLVASÓTERMI PÉLDÁNY
TK 155.285

KFKI-1981-34

P. VÉRTES

FEDGROUP-3 - A PROGRAM SYSTEM FOR PROCESSING EVALUATED NUCLEAR DATA IN ENDF/B, KEDAK OR UKNDL FORMAT TO CONSTANTS TO BE USED IN REACTOR PHYSICS CALCULATION

Hungarian Academy of Sciences

CENTRAL RESEARCH INSTITUTE FOR PHYSICS

BUDAPEST

2017

KFKI-1981-34

FEDGROUP-3 - A PROGRAM SYSTEM FOR PROCESSING EVALUATED NUCLEAR DATA IN ENDF/B, KEDAK OR UKNDL FORMAT TO CONSTANTS TO BE USED IN REACTOR PHYSICS CALCULATION

P. Vértes

Central Research Institute for Physics
H-1525 Budapest 114, P.O.B. 49, Hungary

HU ISSN 0368 5330
ISBN 963 371 815 5

ABSTRACT

A new, completely rewritten version of the FEDGROUP program system [1] is presented in this report. The formulae and the algorithm underlying the calculation are revised. The FEDGROUP-3 is able to calculate group averaged infinite diluted and screened cross-sections, elastic and inelastic transfer matrices, point-wise cross-section sets from evaluated data in ENDF/B, KEDAK and UKNDL format. The program system is written mainly in FORTRAN-IV of IBM-OS, but it can be adepted relatively easily to other type of computers.

АННОТАЦИЯ

В отчете представлен новый, полностью переработанный вариант программной системы FEDGROUP. FEDGROUP-3 рассчитывает среднегрупповые сечения, экранированные и в бесконечном разбавлении, точечные сечения и матрицы упругого и неупругого перехода из оцененных ядерных данных, находящихся в формате ENDF/B, KEDAK и UKNDL. Система программ написана в основном на языке ФОРТРАН-IV для ЭВМ ЕС-1040.

KIVONAT

A report a FEDGROUP programrendszer egy uj teljesen átirt változatát mutatja be. A FEDGROUP-3 végtelen higitásu és leárnyékolt hatáskeresztmetszet átlagokat, pontonkénti hatáskeresztmetszeteket, elasztikus és inelasztikus csoportátmeneti mátrixokat számol ENDF/B, KEDAK illetve UKNDL formátuma nukleáris adatokból. A programrendszer R-40-es számitógépre, legnagyobb részt FORTRAN-IV programozási nyelven iródott.

TABLE OF CONTENT

1. PRINCIPLES OF NUCLEAR DATA PROCESSING BY FEDGROUP-3

1.1 INTRODUCTION

Over the last six years the program system FEDGROUP-2 [1] has come into operation in several laboratories of central and east-European countries. It has been used successfully for processing evaluated data files in KEDAK [2], UKNDL [3], and LENDL [4] format. Its application to files in general ENDF/B format was also attempted but serious problems, arising from the specific structure of these files could not be overcome satisfactorily in the frame of FEDGROUP-2. Most of these problems are connected with the representation of cross-section as a sum of resonance cross-section and background cross--section accepted in the ENDF/B file [4].

For some types of calculation (e.g. Monte Carlo), point-wise cross-sections are required. FEDGROUP-2 could satisfy this requirement but only in a complicated way.

The computer facilities at our disposal have also changed in this period. Computers of the EC-1040 type, using IBM-OS/360, have been installed in various CMEA countries. The new program system FEDGROUP-3 has been developed primarily for this type of computer.

In FEDGROUP-3 the shortcomings of FEDGROUP-2 have been eliminated. The well-proved method of processing used in FEDGROUP-2 is retained but the program organization has been changed too large extent and the calculational routines were completely revised and many of them have been newly written. In the next few sections this method of processing is outlined.

In the second part of this report formulae for the group constants and the methods of calculation are quoted. The third part is a user manual. All details required for the running of this system are included here. In the fourth part the results of test calculations and their comparison with those of other similar codes are discussed, in order to verify our programs. In the fifth part some examples of FEDGROUP calculation (input cards) are presented.

By developing FEDGROUP-3 the experience gained with FEDGROUP-2 has been used to a large extent. This experience has been resulted from the contribution of specialists of 7 countries: Bulgaria, Czechslovakia, the German Democratic Republic, Hungary, Poland, USSR and Yugoslavia.

1.2 COMPONENTS OF THE FEDGROUP SYSTEM

The FEDGROUP system consisted of closely linked files and programs. A file may be either of card-image or of internal type. The outgoing evaluated data files are in card-image form. They are well-known. The concept of internal files is to be explained here.

An internal file consists of unformatted records with equal length - LC. LC is called the buffer length and is given in machine words. The items of the internal file are placed in these records continuously as if the whole file were one large field. The buffer length LC has nothing to do with the structure of the library represented on the file. An item may be placed or retrieved by its address which is a pointer value i.e. the serial number of word counted from a given place of the file. If this place is right at the beginning of the file, then it is said that this address is absolute, otherwise it is an address relative to a given place. There are specially developed subroutines which place or retrieve an item into/from the library by its absolute address. From address the serial number of the record containing the place of the required item is calculated, and the record will be read into (if it is not already in) the fast memory, i.e. into the buffer field of length LC. Actually I/O operation occurs only when an item belonging to a record which is not in the buffer is referred. The larger the buffer length the less I/O operations occur. However, a buffer may use a considerable part of the fast memory. In FEDGROUP it is possible to use at most two internal files at the same time. When an internal file is prepared special care should be taken to output the last record.

Two kinds of internal files have been introduced, viz.

(1) RFOD - this is the working file for evaluated data. When processing evaluated data to group constant this file is used as input.

It is composed of the following parts:

- comment: the only literal part which may give some relevant information to be specified at the time of producing the RFOD
- table of contents (ToC) - list of materials and the related types in RFOD
- data headings (DHs) - detailed information on data sets
- data - a contiguous flow of data

The ToC contains addresses of DHs and one DH contains address(es) for the data set(s). When processing data set(s) the corresponding DH(s) is (are) contained in the fast memory.

A more detailed description of the RFOD format is given in 3.1. The possible DHs and related data structures are described in 3.2.

An RFOD may be prepared from evaluated nuclear data by means of the program PRAFO. However, RFOD may be resulted from RFOD either by the program RFODS performing manipulation with RFOD file, or by processing it to point-

-wise cross-sections by means of the NWZ-3 program. The last possibility is a new feature of FEDGROUP-3 compared with FEDGROUP-2. The RFOD produced by NWZ-3 contains some data types which cannot be contained by an RFOD resulting from a PRAFO run.

(2) SFGK - this is an output format for group constants produced by the NWZ-3 program. It consists of a contiguous series of SFGK sets described in detail in 3.8. Any SFGK set begins with a literal constant 'BEGN' and the whole file ends with the literal 'END'. There are no pointers and table of contents for SFGK sets. In order to facilitate the group constant transmission a BCD card-image format for SFGK file is specified (see 3.8).

Further components of the FEDGROUP system are the following five programs.

EVDAUT - a PL/1 program for manipulation with card-image data files. It may copy selected segments from the whole data tape to a file which is immediately used by PRAFO. Selected cards may be printed out and/or some cards may be changed during the copy, e.g. in order to correct possible errors on the file. The reason for using the PL/1 language for this job is its higher performance. All other programs are written in FORTRAN-IV

PRAFO - a program for preparing RFOD from evaluated data being in card-image evaluated data file. It is developed for KEDAK, UKNDL and ENDF/B data. It is possible to include any user developed PRAFO for data in other formats.

RFODS - is a program for manipulation with RFOD(s). It can give information on a RFOD's content or it can copy selected parts of RFODs to a new RFOD.

NWZ-3 - is the central program of the system. It uses evaluated data in RFOD format and calculates group constants for any user-specified group system and averaging spectrum, or it calculates point-wise cross-sections. The group-constants calculated by NWZ-3 will be given in SFGK format; the point-wise cross-sections will appear in RFOD format. In NWZ-3 there are 10 calculational blocks performing different types of calculations. They are described in 3.6

SFGKS - is a program for manipulation with SFGK sets. It can give information on the SFGK file and sets, merge SFGK sets in order to get group contants for all group in one set. (Due to machine time and fast memory considerations it is not always recommended that the group constants for the whole group system be calculated in one run). SFGKS can reorganize SFGK file by copying selected SFGK sets.

In Fig. 1 the scheme of FEDGROUP-3 is shown i.e. files and programs linked with each other.

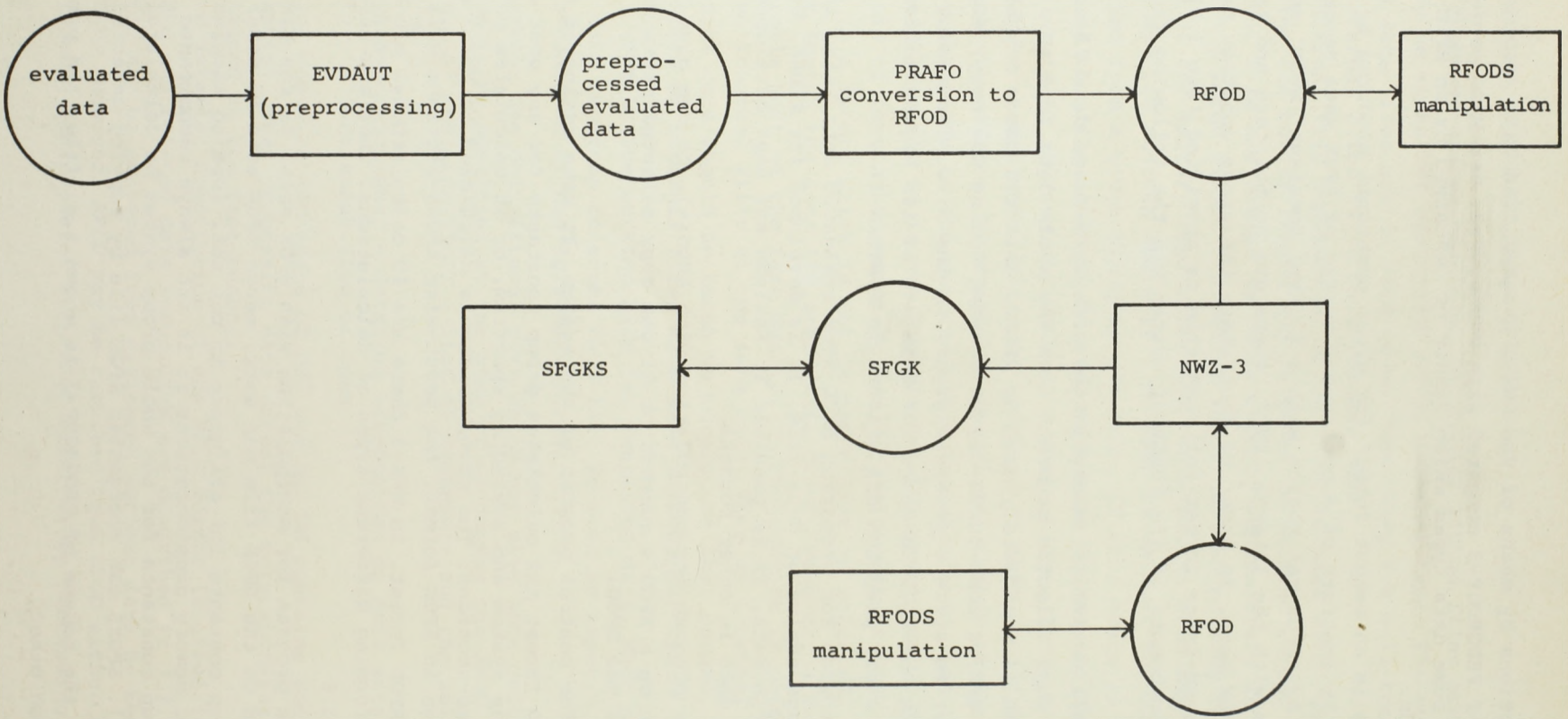


Fig. 1: FEDGROUP is scheme

The FORTRAN programs in the FEDGROUP system are dynamically programmed, i.e. a large field defined in the main program is given over to the formal parameter list of subroutines using large optional data sets. The length of this field is called the dynamic length. The required dynamic length depends on the length of the data set to be processed and on the way of processing. There is a tendency in FEDGROUP to minimize the core memory to be used; because of this when ever possible only those parts of the data set should be retained in the dynamic field which are essential for effective processing. The term "effective" means that there is a definite compromise between the core usage and other parameters (computing time, channel time etc.) of efficiency.

2. FORMULAE AND ALGORITHM USED IN FEDGROUP-3

2.1 DEFINITION OF INFINITE DILUTED AND SELF-SHIELDED GROUP-AVERAGED CROSS-SECTION

Notation:

$\phi(E)$ - averaging flux

$\sigma_t(E)$ - total cross-section

$\sigma_x(E)$ - (n,x) reaction cross-sections

$\langle\sigma\rangle_\infty^i$ - infinite diluted group-averaged cross-section for group i

$\langle\sigma(T,\sigma_o)\rangle^i$ - group-averaged self-shielded cross-section for group i

ϕ_i - group averaged flux for group i

E_i, E_{i+1} - upper and lower boundaries, respectively, of the group i

T - temperature

σ_o - average total background cross-section

The formulae are

$$\phi_i = \int_{E_{i+1}}^{E_i} dE\phi(E) \qquad (2.1.1a)$$

$$\langle\sigma_x\rangle_\infty^i = \frac{\int_{E_{i+1}}^{E_i} dE\phi(E)*\sigma_x(E)}{\phi_i} \qquad (2.1.1b)$$

$$\langle\sigma_t\rangle_\infty^i = \frac{\int_{E_{i+1}}^{E_i} dE\phi(E)*\sigma_t(E)}{\phi_i} \qquad (2.1.1c)$$

$$\langle\phi(T,\sigma_o)\rangle^i = \int_{E_{i+1}}^{E_i} dE\, \frac{\phi(E)}{\sigma_q(E)+\sigma_o} \qquad (2.1.2a)$$

$$\langle\sigma_x(T,\sigma_o)\rangle^i = \frac{\int_{E_{i+1}}^{E_i} dE \, \frac{\phi(E)\sigma_x(E)}{\sigma_q(E)+\sigma_o}}{\langle\phi(T,\sigma_o)\rangle^i} \qquad (2.1.2b)$$

$$\langle\sigma_t(T,\sigma_o)\rangle^i = \frac{\int_{E_{i+1}}^{E_i} dE \, \frac{\phi(E)}{\sigma_q(E)+\sigma_o}}{\int_{E_{i+1}}^{E_i} dE \, \frac{\phi(E)}{(\sigma_t(E)+\sigma_o)(\sigma_q(E)+\sigma_o)}} - \sigma_o \qquad (2.1.2c)$$

where

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

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 resonance according to the theory of Goldstein [16].

The latter is calculated by means of an approximation introduced by Forti [17]

$$\gamma_r = \begin{cases} 1 - 0.5\,\frac{\Gamma_p}{\alpha E_r} & \text{if } \alpha \geq \frac{\Gamma_p}{E_r} \\ 0.5\,\frac{\alpha E_r}{\Gamma_p} & \text{if } \alpha \leq \frac{\Gamma_p}{E_r} \end{cases}$$

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

$$\Gamma_p = \Gamma\sqrt{\frac{\lambda\!\!\!^{-2}}{R^2 E_r}\,\frac{\Gamma_n}{\Gamma} - 1}\,^*$$

$\lambda\!\!\!^-$ - reduced wave-length; R - nuclear radius; Γ, Γ_n - total and neutron width, respectively; E_r - resonance energy.

The narrowness of resonances in a group interval can be characterized by a group averaged value, defined as

---

*In FEDGROUP-2 Γ was used instead of Γ_p - mistakenly - as was noted by A. Trkov. (Institute J. Stafan, Ljubljana, Yugoslavia)

$$\gamma_i = \frac{\int_{E_{i+1}}^{E_i} dE\ \phi(E) \sum_r \gamma_r \sigma_{s_r}(E)}{\int_{E_{i+1}}^{E_i} dE\ \sigma_s(E)\phi(E)}$$

where $\sigma_s(E)$ is the scattering cross-section, NR(E) is the number of resonances taken into account at energy E.

2.2 METHOD OF NUMERICAL INTEGRATION FOR POINT-WISE GIVEN CROSS-SECTION

The formulae given in 2.1 require the numerical evaluation of the integral

$$\int_a^b dX\ \phi(X)*\sigma(X) \qquad (2.2.1)$$

Let $\sigma(X)$ be given at the points $X_1 \leq a \leq X_2 \ldots \leq X_{n-1} \leq b \leq X_n$ and between these points it is determined by certain interpolation rule as

$$\sigma(X) = f(X, X_i, X_{i+1}, \sigma_i, \sigma_{i+1}) \qquad (i = 1, \ldots n-1)$$

where $\sigma_j = \sigma(X_j)$. Thus the integral (2.2.1) is changed to

$$\sum_{i=1}^{n-1} \int_{X_i}^{X_{i+1}} dX\ f(X, X_i, X_{i+1}, \sigma_i, \sigma_{i+1})\phi(X) \qquad (2.2.2)$$

$\phi(X)$ may be given by formula or point-wise. In the latter case let $\phi(X)$ be given at the points $X'_1 \leq a < X'_2 \ldots \leq X'_{m-1} \leq b < X'_m$ and on merging the two point sets, the integral in (2.2.2) can be given as

$$\sum_{k=1}^{L-1} \int_{X_k}^{X_{k+1}} dX\ g(X, X_k, X_{k+1}, \phi_k, \phi_{k+1})*f(X, X_k, X_{k+1}, \sigma_k, \sigma_{k+1}) \qquad (2.2.3)$$

where g denotes an interpolation rule specified for the point-wise flux. In any case ϕ*f or g*f is an analytically given function and the calculation of the relevant integral is performed by Romberg's procedure which is, briefly, the following.

Let

$$I = \int_b^a dx q(x)$$

This integral can be approximated by

$$I_{o,n} = (0.5*(q(a)+q(b))+\sum_{k=1}^{2^n-1} q(x_k^n))*\Delta x_n$$

where

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

and

$$x_k^n = a+k*\Delta x_n.$$

Obviously

$$I_{o,n+1} = 0.5*I_{o,n}+\Delta x_{n+1}\sum_{k=1,3,..}^{2^{n+1}-1} q(x_k^{n+1})$$

Taking the following recurrence relation

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

it is easy to prove that $|I-I_{m,n}| \sim (\Delta x_n)^m$, that is, $I_{n,n}$ is the best approximation for a given n. The criterion of the covergence is

$$|1-I_{n-1,n-1}/I_{n,n}| \leq EPS$$

where EPS is a user specified error limit.

The convergence is fast enough if q(x) is a smooth function. To avoid any waste of computing time an upper limit for n (NUJM) is introduced. On reaching this limit an error message like "NO CONVERGENCE IN..." will be given. It is generally observed that NUJM $\geq$ 4 all cases gives an satisflying level of accuracy disregarding the error message. This means that the contribution of intervals, where there is no convergence, to the whole integral is in most cases small.

2.3 CROSS-SECTIONS IN THE RESONANCE REGION

At present FEDGROUP-3 can process single and multilevel Breit-Wigner resonance parameters to group constants or to point-wise cross-sections. The formulae to be used are in accordance with those included in the publication BNL-102 [4]. Differences between KEDAK and ENDF/B representation are eliminated through PRAFO.

The Doppler-broadened formulae for resolved multilevel Breit-Wigner resonances are

$$\sigma_t(E,T) = \sum_{\ell} \sigma_t^{\ell}(E,T) \qquad (2.3.1a)$$

$$\sigma_x(E,T) = \sum_{\ell} \sigma^{\ell}(E,T) \qquad (2.3.1b)$$

where

$$\sigma_t^{\ell}(E,T) = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_{\ell} + \sum_r \sum_j \sigma_{oc}^r[\psi_r(E,T)\cos 2\delta_{\ell} + \chi_r(E,T)\sin 2\delta_{\ell} + \psi_r(E,T)\alpha_r - \chi_r(E,T)\beta_r] \qquad (2.3.2a)$$

$$\sigma_x^{\ell}(E,T) = \sum_r \sum_j \sigma_{ox}^r \psi_r(E,T) \qquad (2.3.2b)$$

ℓ - orbital angular momentum

j - compound nucleus spin

$$k = 2.196771*10^{-3} \frac{AW}{1+AW} \sqrt{E} \qquad (2.3.3)$$

in the case of the ENDF/B file, and

$$k = \frac{\sqrt{E}}{\lambda_o}$$

for the KEDAK file, where λ_o is the reduced wave-length specified in this file, AW is the ratio of the mass of the particular isotope to that of the neutron.

$$\sigma_{oc}^{r_j} = \frac{4\pi}{k^2} g_j \frac{\Gamma_{nr}(E)}{\Gamma_r(E)} \qquad (2.3.4a)$$

$$\sigma_{ox}^{r_j} = \frac{4\pi}{k^2} g_j \frac{\Gamma_{nr}(E)*\Gamma_x^r}{\Gamma_r^2(E)} \qquad (2.3.4b)$$

$$g_j = \frac{(2*j+1)}{2*(2*I+1)}$$

I is the target nucleus spin

$$\Gamma_{nr}(E) = \frac{P_{\ell}(E)}{P_{\ell}(|E_r|)} \Gamma_{nr}(|E_r|) \qquad (2.3.5a)$$

$$\Gamma_r(E) = \Gamma_{nr}(E) + \Gamma_{\gamma}^r + \Gamma_f^r \qquad (2.3.5b)$$

$$P_o(E) = \rho \qquad (2.3.6a)$$

$$P_1(E) = \frac{\rho^3}{1+\rho^2} \qquad (2.3.6b)$$

$$P_2(E) = \frac{\rho^5}{9+3\rho^2+\rho^4} \qquad (2.3.6c)$$

$\rho = k^*a$ and a is the channel radius (in units of 10^{-12}) and is defined as

$$a = [1.23*(AW)^{1/3} + 0.8)*10^{-1}$$

The phase shifts δ_ℓ are

$$\delta_o = \hat{\rho}$$

$$\delta_1 = \hat{\rho} - \arctan \hat{\rho}$$

$$\delta_2 = \hat{\rho} - \arctan \frac{3\hat{\rho}}{3-\hat{\rho}^2}$$

where $\hat{\rho} = k^*\hat{a}$ and $\hat{a}$ is the effective scattering radius given on the KEDAK and ENDF/B files and contained in the RFOD as the second item of the type 459 (see section 3.3). In the KEDAK formulae [5] $a = \hat{a}$ is taken and this leads to a small inaccuracy in the case ℓ=1 and 2.

For negative resonances in the case of KEDAK, $P_\ell(1.)$ is recommended instead of $P_\ell(|E_r|)$ in formula (2.3.5a). Therefore the Γ_n for ENDF/B data is changed according to

$$\Gamma_n \rightarrow \frac{P_\ell(1.)}{P_\ell(|E_r|)} \cdot \Gamma_n$$

and in the NWZ-3 program the corresponding modification of formula (2.3.5a) is used.

The shift of resonance energy is neglected in all cases.

The other quantities in formulae (2.3.2) are

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

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

$$\theta = \Gamma_r \sqrt{\frac{AW}{4\bar{k}T.E}}$$

($\bar{k}$ is Boltzmann's constant)

$$x = \frac{2(E-E_r)}{\Gamma_r} \qquad y = \frac{2(E'-E_r)}{\Gamma_r}$$

If $T \to 0$ then

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

The terms with α_r and β_r give approximately the multilevel correction to the Breit-Wigner formula [6] where

$$\alpha_r = 0.5^* \sum_{s \neq r} \frac{\Gamma_{sn}(|E_s|)^*(\Gamma_s(|E_s|)+\Gamma_r(|E_r|))}{D_{sr}}$$

$$\beta_r = \sum_{s \neq r} \frac{\Gamma_{sn}(|E_s|)^*(E_s-E_r)}{D_{sr}}$$

$$D_{sr} = (E_s-E_r)^2 + 0.25^*(\Gamma_s(|E_s|) + \Gamma_r(|E_r|))^2$$

The sums are extended over resonances with the same ℓ and j.

The single level Breit-Wigner formula can be got from (2.3.2a) if $\alpha_r = \beta_r = 0$ is taken.

2.4 NUMERICAL PROCEDURES IN THE REGION OF RESOLVED RESONANCES

The rigorous calculation of temperature dependent cross-sections from resolved resonance parameters is a very time consuming process. Therefore some neglections are made which can be verified numerically.

For a given energy point only 1+2*NRES resonances are taken into account: NRES below the energy point and NRES+1 above the energy point. NRES is an input parameter (default=10). Moreover, from these resonances not all taken into account exactly. Only M+1 resonances on both sides of an energy point are taken into account exactly, where M is an input parameter (default=2). This can be understood in the following way. The energy region is divided into sub-intervals by taking the following: resonance energies, E_r, points $E_r \pm 3^*\Gamma_r$, where Γ_r is the total width and $0.5^*(E_r^i+3^*\Gamma_r^i+E_r^{i+1}-3^*\Gamma_r^{i+1})$ and, of course, the end points of the integration interval. For the end points of each sub-interval the cross-sections are calculated in both ways: exactly, i.e. taking into account all resonances and approximately, taking into account M+1 resonances on both sides (that is 2+2*M resonances). The differences of the two results are regarded as linearly interpolable quantities. Inside the interval only 2+2*M resonances are taken into account and the result is corrected by the above specified differences making use of linear interpolation.

For large x the Doppler broadening functions $\psi(x,\theta)$ and $\chi(x,\theta)$ go over to their asymtotic form. The boundary point: EZ. This is an input parameter (default=100.)

Sometimes it may occur that the elastic cross-section calculated from the resonance parameters becomes negative at certain energy points. If no background correction to be added is defined on the evaluated data file (e.g. KEDAK file) then the negative value is corrected as $\sigma_n(E)=SMIN*\sigma_{pot}$, where σ_{pot} is the potential cross-section and SMIN is an input parameter (default=0.1).

If a linearly interpolable cross-section set is required then the calculation is performed in the following way. The sub-interval, mentioned above, is halved and investigated to see whether the relative deviation of calculated and linearly interpolated values is less then EPS (input value, default the = 0.01). If not then the halving process is continued otherwise the next sub-interval is taken. In order to save space and computing time the number of points is maximalized as $2^{NUJM}+1$ where NUJM is an input parameter (default=10).

If group constants are required then Romberg's integration procedure is applied to each sub-interval. This is essentially also an interval halving method.

The described method of generation of resonance cross-section sets is very economic. In this way a given accuracy can be reached by a minimum number of energy points. There is however a less economic but more straighforward way: division of the required energy interval into lethargy equidistant subintervals.

It should be noted that in spite of the correction of negative cross--section values performed with SMIN, negativ resonance cross-sections may occur. This is due to the approximation concerning the neighbouring resonances. By increasing the parameter M, the negative scattering cross-sections will be eliminated.

2.5 CALCULATION OF CROSS-SECTION IN UNRESOLVED RESONANCE REGION

The formalism used in FEDGROUP-3 is mainly based on the formalism used in MIGROS-3 [5] but taking into account that in ENDF/B there is no recommendation for overlapping correction. There are three cases for unresolved resonance parameters specification.

- only energy independent parameters are given
- energy independent and energy dependent parameters are given
- only energy dependent parameters are given

The first case may occur both for KEDAK and ENDF/B data. The second case is valid only for KEDAK, the third one only for ENDF/B data. As ENDF/B does not reommend any overlapping correction, this correction is omitted in

the third case and it can be made by request in the first one.

The formulae for cross-sections averaged over an interval ΔE around energy E^* are

$$\sigma_x(E^*) = \sum_s \sigma_x^s(E^*) \qquad (2.5.1a)$$

$$\sigma_t(E^*) = \sum_\ell (2\ell+1)\frac{4\pi}{k^2(E^*)}\sin^2\delta_\ell + \sum_s \sigma_r^s(E^*) = \sigma_{pot} + \sum_s \sigma_r^s \qquad (2.5.1b)$$

where s means ℓ, j pair of indices.

$$\sigma_x^s(E^*) = \frac{2\pi^2}{k^2(E^*)} g_j \frac{1}{D^s(E^*)} \left\langle \frac{{}^s\Gamma_n \, {}^s\Gamma_x}{{}^s\Gamma} \right\rangle \qquad (2.5.2a)$$

$$\sigma_r^s(E^*) = \frac{2\pi^2}{k^2(E^*)} g_j \frac{1}{D^s(E^*)} \bar{\Gamma}_n^s \cos 2\delta_\ell \qquad (2.5.2b)$$

In the following the argument E^* will be omitted. The screened cross-sections, according to Froehlich's theory with Huschke's modifications [5], are

$$\sigma_x(T,\sigma_o) = {}^s\sigma_{p,eff} \frac{(1+\frac{\sigma_r^s}{\sigma_t+\sigma_o}) \frac{\langle \Gamma_x^s \cdot J(\beta^s,\theta^s)\rangle}{D^s \cos 2\delta_\ell} - \frac{D^s \sigma_x^s \sigma_r^s}{\Delta\sqrt{2\pi}(\sigma_t+\sigma_o)^2}\cdot\varepsilon}{R} \qquad (2.5.3a)$$

$$\sigma_t(T,\sigma_o) = {}^s\sigma_{p,eff} \frac{(1+\frac{\sigma_r^s}{\sigma_t+\sigma_o}) \frac{\langle \Gamma^s \cdot J(\beta^s,\theta^s)\rangle}{D^s} - \frac{D^s \sigma_r^s \cdot \sigma_r^s \cdot \varepsilon}{\Delta\sqrt{2\pi}(\sigma_t+\sigma_o)^2}}{R} \qquad (2.5.3b)$$

$$R = 1 - (1+\frac{\sigma_r^s}{\sigma_t+\sigma_o}) \frac{\langle \Gamma^s \cdot J(\beta^s,\theta^s)\rangle}{D^s} + \frac{D^s \sigma_r^s \cdot \sigma_r^s \cdot \varepsilon}{\Delta\sqrt{2\pi}(\sigma_t+\sigma_o)^2} \qquad (2.5.3c)$$

$${}^s\sigma_{p,eff} = \sigma_t + \sigma_o - \sigma_r^s$$

$$\beta^s = \frac{\sigma_t+\sigma_o}{4\pi g_j \cos 2\delta_\ell} k^2 \frac{\Gamma^s}{\Gamma_n^s}$$

$$\theta^s = \frac{\Gamma_s}{\Delta} , \qquad \Delta = \sqrt{\frac{4\bar{k}T^*E^*}{AW}}$$

$\bar{k}$ is the Boltzmann Constant

$$J(\beta,\theta) = \int_0^\infty \frac{\psi(\theta,x)}{\psi(\theta,x)+\beta}\, dx$$

If T=O. then ε=O. For Doppler broadened resonances ε is determined by formulae (5.24) and (5.25) of [5]. It is tabulated as a function of D^s/Δ and in the program this table is used with proper interpolation.

Without overlapping correction, formulae (2.5.3) become

$$\sigma_x^s(T,\sigma_o) = (\sigma_{pot} + \sigma_o) \frac{<\Gamma_x^s J(\beta^s,\theta^s)>}{D^s \cos 2\delta_\ell * R} \qquad (2.5.4a)$$

$$\sigma_t^s(T,\sigma_o) = (\sigma_{pot} + \sigma_o) \frac{<\Gamma^s J(\beta^s,\theta^s)>}{D^s R} \qquad (2.5.4b)$$

$$R = 1 - \frac{<\Gamma^s J(\beta^s,\theta)>}{D^s} \qquad (2.5.4c)$$

$$\beta^s = \frac{\sigma_o+\sigma_{pot}}{4\pi g_j \cos 2\delta_\ell} \cdot k^2 \frac{\Gamma^s}{\Gamma_n^s}$$

The bracket <> in the above formulae means an averaging over a probability distribution. It is assumed that Γ_n and Γ_f are distributed according to a χ^2 distribution, that

$$F(\Gamma)d\Gamma = \frac{\nu}{2\bar{\Gamma}G(\frac{\nu}{2})} \left(\frac{\nu}{2}\frac{\Gamma}{\bar{\Gamma}}\right)^{\frac{\nu}{2}-1} \exp\left(-\frac{\nu}{2}\frac{\Gamma}{\bar{\Gamma}}\right) d\Gamma$$

where ν degree of freedom, $\nu=\nu_n$ for Γ_n and $\nu=\nu_f$ for fission width. Radiation width, because of the high degree of freedom is constant. The integration over the distribution is performed numerically in the same way as done in MIGROS-3 [5].

The average Γ_n width is calculated from the average reduced neutron width by the formula [4]

$$\bar{\Gamma}_{n_{\ell,j}} = \Gamma^o_{n_{\ell,j}} \sqrt{E}\, V_\ell(E)\, \nu_{n_{\ell,j}}$$

where

$$V_\ell(E) = \frac{P_\ell(E)}{\rho}$$

$P_\ell(E)$ and ρ are defined in section 2.3.

It should be noted that for KEDAK data the formula

$$\bar{\Gamma}_{n_\ell,j} = \Gamma^o_{n_\ell,j} \sqrt{E}\, V'_\ell(E)$$

is recommended, where $V'_\ell(E)$ is defined similarly to $V_\ell(E)$ but instead of channel radius 'a' the effective scattering radius 'â', specified on the evaluated data file is used.

There is a similar problem with the energy dependence of the average level density. The formalism recommended for KEDAK data [5] defines a slight energy dependence using formula

$$s_{D(E)} = s_{\bar{D}_o} \frac{(E_b+E)^2}{E_b^2} \mathrm{EXP}(-\sqrt{89.72*10^{-6}(E_b+E)} + \sqrt{89.72*10^{-6}E_b})$$

where E_b is the binding energy of the last neutron (library data). In the case of energy independent parameters the ENDF/B specification does not recommend any energy dependence for $s_{\bar{D}}$.

The group constants in the unresolved resonance region can be calculated by averaging the smooth energy dependent cross-sections gained from the unresolved resonance parameters.

2.6 CALCULATION OF ELASTIC SCATTERING MATRIX

Notation:

$\sigma_m^{i\to j}$ - the m-th Legendre momentum of elastic transfer cross-section from group i to group j

$\pi_m(E\to i)$ - the m-th Legendre momentum for elastic scattering probability from energy point E to group i

Formulae:

$$\pi_m(E\to i) = \int_{E_{i+1}}^{E_i} dE' f(E,\mu_c(E/E')) P_m(\mu_L(E/E')) \qquad (2.6.1)$$

$\mu_L(E/E')$ and $\mu_c(E/E')$ cosine of the scattering angle when neutron scattered from energy E to E' (in laboratory and centre-of-mass system, respectively)

According to the slowing-down theory

$$\mu_L(E/E') = \frac{A+1}{2}\sqrt{\frac{E'}{E}} - \frac{A+1}{2}\sqrt{\frac{E}{E'}} \qquad (2.6.2a)$$

$$\mu_c(E/E') = 1 - \frac{(A+1)^2}{2A}\left(1 - \frac{E'}{E}\right) \qquad (2.6.2b)$$

$f(E,\mu_c(E/E'))$ - normalized angular distribution of elastic scattered neutrons in the centre-of-mass system

$P_m(\mu_L)$ - Legendre polynomial of order m.

$$\sigma_m^{i\to j} = \frac{\int_{E_{i+1}}^{E_i} dE\,\phi(E)\,\sigma(E)\,\pi_m(E\to j)}{\int_{E_{i+1}}^{E_i} dE\,\phi(E)} \qquad (2.6.3)$$

$\sigma_s(E)$ is the elastic scattering cross-section.

The course of the calculation is the following. The values $\pi_m(E\to i)$ are calculated from the angular distribution of elastic scattering and stored like primary data i.e. on RFOD. To the same RFOD a set of point-wise elastic scattering cross-sections is written on covering energy interval which overlaps the energy interval covered by $\pi_m(E\to i)$. By means of this RFOD the $\sigma_m^{i\to j}$ matrix is calculated.

$\pi_m(E\to i)$ may differ from zero only in the energy interval $E_i\alpha>E>E_{i+1}$,

where

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

On RFOD, $\pi_m(E\to i)$ are given only for this energy range.

2.7 CALCULATION OF SLOWING DOWN CONSTANTS

According to the theory developed in [7] the constants to be used in the Goertzel-Greuling equations may be derived from

$$Q_{m,n}^j = \frac{\frac{2\pi}{n!}\int_{E_{j+1}}^{E_j} dE\,\phi(E)\int_{-1}^{-1} d\mu_c P_m(\mu_L)\,(\log W(\mu_c))^n\, f(\mu_c,E)}{\int_{E_{j+1}}^{E_j} dE\,\phi(E)} \qquad (2.7.1)$$

where

μ_L is the scattering angle in the laboratory system

μ_c is the scattering angle in the centre-of-mass system

$f(\mu_c,E)$ - normalized angular distribution of elastic scattered neutrons

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

E - energy before scattering

E' - energy after scattering

A = atomic mass/neutron mass

$P_m(\mu)$ - Legendre polynomial of order m

For any materials the following Goertzel-Greuling constants are used:

$\mu^j = Q^j_{1,0}$ - average scattering cosine in group j (2.7.2a)

$\xi^j = -Q^j_{0,1}$ - average lethargy change in group j (2.7.2b)

For atoms having mass less than a certain limit AM, the following constants are yet needed:

$$\xi^*_j = \xi_j\left(1 - \frac{\Lambda_o(E_j)/E_j - \Lambda_o(E_{j+1})/E_{j+1}}{E_j - E_{j+1}}\right) \tag{2.7.2c}$$

$$\Gamma_j = \int_{E_{j+1}}^{E_j} dE\phi(E)\Lambda_o(E) \Big/ \int_{E_{j+1}}^{E_j} dE\phi(E) \tag{2.7.2d}$$

$$H_j = Q^i_{1,1} \cdot \left(1 - \frac{\Lambda_1(E_j)/E_j - \Lambda_1(E_{j+1})/E_{j+1}}{E_j - E_{j+1}}\right) \tag{2.7.2e}$$

$$Z_j = \int_{E_{j+1}}^{E_j} dE\phi(E)\Lambda_1(E) \Big/ \int_{E_{j+1}}^{E_j} dE\phi(E) \tag{2.7.2f}$$

where

$$\Lambda_o(E) = -\frac{\int_{-1}^{1} d\mu_c (\log(W(\mu_c))^2 f(\mu_c, E)}{\int_{-1}^{1} d\mu_c (\log(W(\mu_c)) . f(\mu_c, E)} \tag{2.7.3a}$$

$$\Lambda_1(E) = -\frac{\int_{-1}^{1} d\mu_c \mu_L (\log(W(\mu_c))^2 f(\mu_c, E)}{\int_{-1}^{1} d\mu_c \mu_L \log W(\mu_c) . f(\mu_c, E)} \tag{2.7.3b}$$

In the case of isotropic scattering $f(\mu_c, E) = 0.5$ and the integrals in (2.7.1) can be analytically evaluated as

$$\mu = 2/3\ A \tag{2.7.4a}$$

$$\xi = \xi^* = \frac{(A+1)^2}{4A}\left(1 - \left(\frac{A-1}{A+1}\right)^2 (1+q)\right) \tag{2.7.4b}$$

$$\eta = H = \frac{(A+1)^2}{4A}\left((A+1)/3 \times (2/3 - (2/3+q)e^{-1.5q}) - (A-1)(2-(2+q)e^{-0.5q})\right) \tag{2.7.4c}$$

$$\Gamma = -\frac{(A+1)^2}{4A}\ \frac{1}{2\xi}\ (2 - (2+2q+q^2)e^{-q}) \qquad (2.7.4d)$$

$$Z = -\frac{(A+1)^2}{4A}\ \frac{1}{2\eta}\ \left[\frac{A+1}{3}\ (8/9-(8/9+4/3q+q^2)e^{-q}) - (A-1)(8 - (8+4q+q^2)e^{-q/2})\right] \qquad (2.7.4e)$$

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

Note: In the isotropic case $\Lambda_o(E)$ and $\Lambda_1(E)$ are constants.

2.8 CALCULATION OF INELASTIC TRANSFER MATRIX

The inelastic transfer matrix is composed of $\sigma_{in}^{i\to j} = \sigma_{ind}^{i\to j} + \sigma_{inc}^{i\to j}$ where $\sigma_{ind}^{i\to j}$ is the inelastic group transfer cross-section from discrete excitation levels and $\sigma_{inc}^{i\to j}$ is that from the unresolved levels.

The discrete level inelastic scattering is described by [8]

$$\sigma_{in}^{k}(E\to E') = \sum_k \sigma_{in}^{k}(E)\,\delta(\langle E_k\rangle - E')$$

where

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

where Q_k is the threshold energy of level k.

The discrete level inelastic scattering matrix will be a sum of one level scattering matrices, where a one-level scattering matrix element is

$$\sigma_{ind}^{k,i\to j} = \frac{\int_{E_{ij}}^{E'_{ij}} dE\ \sigma_{in}^{k}(E)\phi(E)}{\int_{E_{i+1}}^{E_i} dE\ \phi(E)}$$

where the interval (E_{ij},E'_{ij}) is the common part of the intervals (E_{i+1},E_i) and (E^k_{j+1},E^k_j)

where

$$E_x^k = \frac{(A+1)^2}{A^2+1}\ (E_x + \frac{A}{A+1}\,Q_k)$$

For the description of the unresolved inelastic scattering the distribution

$$P_i^C(E' \to E) = \begin{cases} C*E*EXP(-E/\theta(E')) & \text{if } 0 \le E \le E' - Q \\ 0 \text{ otherwise} & \end{cases}$$

is used, and [9]

$$\theta(E') = \sqrt{\frac{E'}{T_m * A}}$$

T_m is the nuclear temperature. (Input parameter TMAG, default = 0.16) Q is specified as that first energy point for unresolved inelastic scattering for which $\sigma_{in} \ge 1.0*10^{-10}$ barn. (This corresponds to the threshold of unresolved inelastic scattering). C is a normalization factor.

The transfer matrix elements for unresolved inelastic scattering

$$\sigma_{inc}^{i \to j} = \frac{\int_{E_{i+1}}^{E_i} dE' \sigma_{in}^C(E') \phi(E') P_i^C(E' \to j)}{\int_{E_{i+1}}^{E_i} dE \phi(E)}$$

where

$$P_i^C(E' \to j) = \int_{E_{j+1}}^{E_j} dE \; P_i^C(E' \to E)$$

The last integral can be calculated analytically. If $E_{j+1} < E'-Q$ then

$$P_i^C(E' \to j) = \theta^2(E') \left[e^{-\frac{E_{j+1}}{\theta(E')}} \left(1 + \frac{E_{j+1}}{\theta(E')}\right) - \left(1 + \frac{E_j'}{\theta(E')}\right) e^{-\frac{E_j'}{\theta(E')}} \right]$$

where $E_j' = MIN(E'-Q, E_j)$; If $E_{j+1} \ge E'-Q$ then $P_i^C(E' \to j) = 0$.

In both cases, discrete and unresolved, the accuracy of calculation for high energy degradation, i.e. for lower inscattering group is poor. This could be improved by introducing double precision for certain variables. However, the accuracy of inelastic data does not warrant the usage of a longer and more complicated calculation. With appropriate cut-off the matrix elements for the lower inscattering groups are taken to zero.

3. DETAILED DESCRIPTION OF FEDGROUP-3 FOR USERS

3.1 RFOD'S STRUCTURE

The quoted length values are given in machine words (four bytes in the case of IBM-OS).

The RFOD consists of the following parts:

I Comment part, length=LK+1
LK - length of comment
comment

II Length values, length=4
L1 - length of the whole file
L2 - length of the Table of Contents
L3 - length of data headings
L4 - length of data

III Table of Contents (ToC) length=1+2*NMAT+ $\sum_{i=1}^{NMAT} 2*NTYP_i$
NMAT - number of materials contained in RFOD for each material:
MATN - name of the material
NTYP - number of data types for this material for each type of each material:
NTN - data type name
NA - address of the corresponding data heading (relative to the beginning of data heading's part)

IV Data Headings (DHs)

V Data

The structure and length of parts IV and V are given in section 3.2.
Note: all names used in RFOD are numerical ones; about their specification see later.

3.2 DATA HEADINGS AND DATA STRUCTURE

The first word of a Data Heading is the type format number - NTF. The second word is the length of the remaining part of the DH - NL.

The structure and length of the remaining part of the DH depend on NTF and are given in the following table.

NTF	NL	Data Heading
1	5	NDAT,NAC,NFC,INTA,INTF
5	9	NF,NDAT1,NDAT2,NAC1,NAC2,NFC,INTA1,INTA2,INTF
6	4	NT,NDAT,NAC,NFC
7	4	NT,NDAT,NAC,NFC
8	5	NT,NSI,NDAT,NAC,NFC
10	N	N real numbers
11	L11*	NW,NFN,((FP(J,I),J=1,NW),$NDAT_i$,NAC_i,NFC_i,$INTA_i$,$INTF_i$, I=1,NFN)
20	3	NDAT,NAC,NA
21	L21*	NW,($INTW_i$ I=1,NW),NFN,((FP(J,I),J=1,NW),$NDAT_i$,NFC_i,$INTA_i$, $INTF_i$,I=1,NFN)

L11=2+NFN(NW+5)
L21=2+NW+NFN*(NW+5)

The meaning of notations in the above table is the following:

NDAT,NT,NSI,NF represent data length

NA - length of one sub-set of a data set

NW - number of parameters

NAC,NFC - addresses for argument and function vector, respectively (relative to the beginning of part V)

NFN - number of sub-headings

FP - parameters (real or integer type)

INTW,INTA,INTF - interpolation numbers (see section 3.9)

Any NTF specifies the structure of the corresponding data in part V of RFOD, as given in the following table.

NTF	Data structure
1	ARG(NDAT),FUN(NDAT)
5	ARG(NDAT1),ARG(NDAT2),FUN(NF,NDAT2,NDAT1)
6	T(NT),DAT(NT+1,NDAT)
7	T(NT),DAT(4*NT+1,NDAT)
8	T(NT+NSI),DAT(5+4*NT*NSI,NDAT)
10	no data belong to this type in part V
11	for each sub-heading: ARG(NDAT),FUN(NDAT)
20	DAT(NA,NDAT)
21	for each sub-heading: ARG(NDAT),FUN(NDAT)

Explanation:

ARG - arguments, e.g. energy, scattering angle
FUN - function values, e.g. cross-sections, probability distribution
T - parameters, e.g. temperatures, σ_o values.

3.3 REPRESENTATION OF NUCLEAR DATA ON RFOD

The correspondence between the nuclear data type, type name (NTN) and format type (NTF) is given in the following table. Some of the nuclear data types may be represented by various format types.

NTN	NTF	Description
458	10	1 - A - atomic mass, 2 - Z - atomic order, 3 - RIS - nuclear spin in the ground state
459	10	1 - $\lambda\sqrt{E}$ - reduced wave length, 2 - R - nuclear radius, 3 - EB - binding energy of the last neutron
4511	10	1-2 - EL(2) lower boundaries of the resolved and unresolved resonance regions, respectively: 3-4 - EU(2) upper boundaries of the resolved and unresolved resonance regions, respectively; 5-6 - EFLAG(2) control numbers for resonance calculation (see section 3.6, the description of block 4.)
5152	20	resolved resonance parameters, sub-set's length=10 1 - ER - resonance energy; 2 - AL - orbital angular momentum; 3 - AJ - compound state spin; 4 - G=(2*AJ+1)/2/(2*RIS+1) statistical factor; 5 - Γ - total width 6 - Γ_n - neutron width; 7 - Γ_γ - radiation width; 8 - Γ_f - fission width; 9 - ρ - isotope abundance; 10 - EUP - upper boundary of the resolved resonance region for the given isotope;
5153	20	energy independent unresolved resonance parameters, sub-set's length=8 1 - AL - orbital angular momentum 2 - AJ - compound state spin 3 - Γ_γ average radiation width; 4 - $\bar{D}$ - average level density; 5 - Γ^o - average reduced neutron width; 6 - ν_n - number of degrees of freedom in the neutron width distribution;

NTN	NTF	Description
		7 - ρ - isotope abundance;
		8 - ELM - lower boundary of the unresolved resonance region for this isotope;
5155	20	energy dependent unresolved resonance parameters, sub-set's length=5
		1 - E - energy;
		2 - AL - orbital angular momentum;
		3 - AJ - compound state spin;
		4 - ν_f - number of degrees of freedom in the fission width distribution;
		5 - Γ_f - average fission width;
5155	11	energy dependent unresolved resonance parameters
		NW=2, NFN= $\sum_{AL}$ (number of compound states of different spin)
		Both parameters are integer: ID and NA and they specify the argumentum and function structure as
		ARG(ID) and FUN(NA,NDAT), respectively.
		There are two cases:
		a/ ID=10, NA=6
		The ARG sub-set is:
		1 - AL - orbital angular momentum;
		2 - AJ - compound state spin;
		3 - ν_x - number of degrees of freedom for competitive reaction width;
		4 - ν_n - number of degrees of freedom for neutron width;
		5 - ν_γ - number of degrees of freedom for radiation width;
		6 - ν_f - number of degrees of freedom for fission width;
		7 - RIS - spin of the ground state;
		8 - ρ - isotope abundance;
		9 - ELM - lower boundary of the unresolved resonance region for this isotope;
		10 - IS - the serial number of the isotope
		The FUN sub-set is:
		1 - E - energy:
		2 - $\bar{D}$ - average level spacing

NTN	NTF	Description
		3 - Γ_x - average competitive reaction width; 4 - Γ_n^o - average reduced neutron width; 5 - Γ_γ - average radiation width; 6 - Γ_f - average fission width; b/ ID=13, NA=2 The first ten quantities of the ARG sub-set are the same as in case a/, the next three quantities are: 11 - $\bar{D}$ - average level spacing; 12 - Γ_n^o - average reduced neutron width; 13 - Γ_γ - average radiation width; The FUN sub-set is: 1 - E - energy; 2 - Γ_f - average fission widht;
1251	1	ARG: energy, FUN: average cosine of elastic scattering in the laboratory system;
1251	6	NT=1, DAT: energy and average cosine of elastic scattering in the laboratory system (in one sub-set)
1455	1	ARG: energy, FUN: ν_p - prompt neutron yield per fission;
1461	1	ARG: energy, FUN: χ_p - prompt neutron fission spectrum;
1462	1	ARG: energy, FUN: χ_d - delayed neutron fission spectrum;
456	20	Crainberg spectrum, sub-set's length=4 1 E - energy; 2-4 A,B,C corresponding Crainberg parameters;
1000+n	1	n=MT - reaction type number as defined in ENDF/B ARG: energy, FUN: cross-section values corresponding to MT;
1000+n	6	T: temperature values, DAT: energy and cross-section values corresponding to energy and temperature values (in one sub-set)
1000+n	11	This format is recommended for threshold reactions. NW=1, NFN=1, FP: threshold energy, ARG: energy, FUN: cross-section value;
1000+n	21	This format is recommended for temperature dependent

NTN	NTF	Description
		cross-sections. NW=1, FP=temperature, ARG: energy, FUN: cross-section values;
1005	11	Inelastic level cross-sections NW=1, NFN - number of inelastic levels, FP: excitation energy, ARG: energy, FUN: cross-section values.
1015	1	unresolved inelastic level's cross-section. ARG: energy, FUN: cross-section values
2002	11	Coefficients of Legendre polynomial expansion for angular distribution of elastic scattering. NW=1, NFN: number of energy points, FP: energies ARG: no meaning, FUN: the coeffecients;
2002	21	Tabulated angular distribution for elastic scattering. NW=1, NFN: number of energy points, FP: energies, ARG: cosine of scattering angle, FUN: angular distribution;
4018	1	ARG: energies, FUN: ν - average number of fission neutrons;

The sequencing of data occurs generally according to ascending energy or angle values. However in the case of data consisting of sub-sets, there may be other sequencing parameters, too. This is shown in the next table. (The earlier argument changes more rapidly)

NTN	NTF	Sequencing hierrarchy
5152	20	IS,AJ,AL,E
5153	20	IS,AJ,AL
5155	20	AJ,AL,E

IS - is the serial number of the isotope

By processing of the primary evaluted nuclear data in RFOD format using the NWZ-3 program, point-wise data may be obtained in RFOD format. These data may have the type name and format given in the following table.

NTN	NTF	Original data	Description
NTNAM	7	5152,5153,5155 1001,1002,1018, 1102	Temperature dependent point-wise cross--section for a user specified energy interval. T: temperature values FUN (one sub-set): $E,(\sigma_t(T_i,E),\sigma_\gamma(T_i,E),\sigma_s(T_i,E,),\sigma_f(T_i,E)$, I=1, NT)
NTNAM	8	5153,5155,1001 1002,1018,1102	Temperature dependent self-shielded point-wise cross-sections in the unresolved resonance region, for a user-specified energy interval. T: temperature and σ_o values FUN (one sub-set): $E,\sigma_t^\infty,\sigma_\gamma^\infty,\sigma_s^\infty,\sigma_f^\infty$, $((\sigma_t(T_i,\sigma_o^j,E)$, $\sigma_\gamma(T_i,\sigma_o^j,E),\sigma_s(T_i,\sigma_o^j,E),\sigma_f(T_i\sigma_o^j,E)$, I=1,NT), J=1,NSI)
2002	11	2002	In-group scattering probabilities (see 2.6) NW=2, NFN=NM1*NG, FP: IG - in-scattering group, M - momentum ARG: energy values for which $\pi_o^{IG}(E) > 0$, FUN: in-group-scattering probabilities

NTNAM is the group-constant name specified by user
$\sigma_t,\sigma_\gamma,\sigma_s$, and σ_f denote total, (n,γ), elastic and fission cross-sections, respectively. NM1 is the number of Legendre momenta, NG - number of in--scattering groups.

3.4 THE WORK OF THE PRAFO PROGRAM; INPUT DESCRIPTION

After input of some control numbers and comment text from the input cards, the comment is written into RFOD and the program branches on the subroutine which processes the desired type of evaluated file.

The first card of the first material is retrieved. This occurs in various ways depending on the type of file to be processed. The number of skipped cards (to be specified by input, default=1000) is restricted in order to save computing time in the case when the name for material identification is not given properly. Therefore the preparation of the evaluated file - i.e. the copying of the required segment(s) to a scratch file is inevitable before a PRAFO run.

By finding the required material the data types are read in. Fortunately, each file has a type catalog at the beginning of the material. The names of types are translated and the format type numbers (NTF) are assigned by a dictionary. To any type of file belongs a standard dictionary which can be modified or overriden by input. When a data type is not required to be processed, then NTF=0 is assigned. The types are processed in the same sequence as they are in the file. The ToC and the DHs are compiled in the fast memory, in the dynamic field; the data are written to an auxiliary file. The total length of ToC and DHs should be estimated in advance and given by input (default values are 100 and 500, respectively, which are often not enough). If the resulting ToC or DHs are longer than those given in advance an error message is generated and the processing is terminated.

After finishing the processing of the file, the auxiliary file is closed and rewound. The length values, ToC and DHs are written into the RFOD and the whole content of the auxiliary file is copied after them, and RFOD is closed. Note: the auxiliary file is also a file of internal type, as described in section 1.2.

On request, the table of contents or the whole RFOD can be printed out.

If a new source of evaluated data differs from the existing ones (KEDAK, UKNDL,ENDF/B) then a user can write an adequate PRAFO. How this should be done will be discussed in 3.13.

The input is described in the following tables.

Namelist name: PRAF

Var.name	Default	common name	pos.	Description
NLIB	2	PEIF	3	log.number for RFOD
NAUX	3	PEIF	4	log.number for auxiliary file
NPRAF	-	-	-	control number for file to be processed: 1 - KEDAK, 2 - UKNDL, 3 - ENDF/B, 4 - user-written
NFIL	1	PEIF	5	log. number for evaluated data file
NWORD	18	-	-	length of the comment - LK
LC	900	LCLCLC	1	buffer length
NCOUT	0	-	-	output control number (see later)
LCAT	100	WBND	6	maximum length of ToC
LDH	500	WBND	7	maximum length of DHs

This namelist card should be followed by (NWORD-1)/20+1 cards with the text of comment for RFOD.

Namelist name: MAT

Var.name	Default	Description
LSNM	1000	maximal number of cards which may be skipped before processing
MATF	-	identification number for evaluated data to be processed
MATN	=MATF	identification name on RFOD (to be assigned by FEDGROUP user)
NDICT	0	< 0 the whole standard or previously used dictionary is overriden and a new dictionary is specified by input with |NDICT| entries ≥ 0 default or previously used dictionary is modified with NDICT entries.
NDC	0	> 0 the first NDC entries are used from the dictionary compiled for the previously processed material
EPS**	0.01	accuracy of the data linearization
NUJM**	300	maximum number of points from linearization between two data points
EBLAST***	6.541E6	bounding energy of the last neutron

* MATF=DFN in the case of UKNDL [3], MAT in the case of ENDF/B [4], and 10000*IZ+A for KEDAK where IZ the atomic number and A the rounded value of mass.

** These are not necessary for KEDAK processing

*** Needed only for ENDF/B processing

If |NDICT| > 0 then this namelist card is followed by dictionary entries in free format. A dictionary entry consists of three integers

1 - type name on the original file,
2 - type name on the RFOD
3 - NTF, to be assigned

After the last processed material a namelist card with MATF=-1 follows, in order to close the processing.

Values of output control number: (NCOUT=Σ k)

k	output action
1	output of the input namelist cards
2	only short information on the compiled RFOD,*
6	print the whole compiled RFOD*
16	print the first and last data point for each data set

*These are mutually exclusive

3.5 STANDARD DICTIONARIES FOR THE FILES KEDAK, UKNDL AND ENDF/B

KEDAK Number of entries: 22

KEDAK name	RFOD name	NTF	KEDAK name	RFOD name	NTF	KEDAK name	RFOD name	NTF
14511	4511	10	14580	458	10	14560	456	20
21520	5152	20	21530	5153	20	21550	5155	20
30010	1001	1(6)	30020	1002	1(6)	30030	1003	1(6)
30040	1004	1	30050	1005	11	30051	1015	1
30160	1016	1	30190	1018	1(6)	31020	1102	1(6)
34520	4018	1(6)	34550	1455	1	34610	1461	1
34620	1462	1	32510	1251	1(6)	14590	459	10
40022	2002	21						

The NTF numbers in parantheses refer to an alternative way of processing which can be specified by input. They are recommended then when the data set is large.

UKNDL Number of entries: 24

UKNDL name	RFOD name	NTF	Remark
1000+I	1000+I	1(6)	I=from 1 to 4,15,18,101,102,103,107
1000+I	1000+I	11	I=16,17
1000+I	1005	11	I=from 5 to 14
2002	2002	21	
4018	4018	1	

The NTF numbers in parantheses refer to an alternative way of processing which can be specified by input. They are recommended then when a linearly interpolable set is required e.g. for numerical Doppler broadening.

ENDF/B Number of entries: 17

ENDF/B name	RFOD name	NTF	ENDF/B name	RFOD name	NTF	ENDF/B name	RFOD name	NTF
1451	458	10	1451	459	10	1451	4511	10
2151	5152	20	2151	5153*	20	2151	5155*	11
3001	1001	1	3002	1002	1	3003	1003	1
3004	1004	1	from	3051 up	to	3090	1005	11
3091	1015	1	3016	1016	1	3018	1018	1
3102	1102	1	3251	1251	1	4002	2002	11 or 21

*5153 and 5155 are mutually exclusive types

The original name of data on the ENDF/B file consists of the file number NF and the reaction type number MT:

name=1000*NF+MT

In some cases to one ENDF/B type corresponds more then one types on RFOD.

3.6 CALCULATIONAL BLOCKS OF THE NWZ-3 RPOGRAM

A calculational block is called from a control routine named CALCF3 by specifying its number of the TYPE namelist card for parameter NFEL. The name and the formal parameter list of a calculational block are quite typical. The name is always F3BLOn, where n is the number of the calculational block, and the formal parameter list is the following:

For blocks from 1 to 6:

IPAS1(..), IPAS2(..),...	- the data headings of nuclear data to be used
EG(..)	- the group boundaries
EF(..),FL(..)	- energy points and corresponding spectrum values in ascending order
WORK(...)	- working field
LFR	- length of the working field
BFG(..),BFK(..)	- buffer field for RFOD and SFGK, respectively.

For blocks from 7 to 10:

IPAS1(..),IPAS2(..),...	- the data headings of nuclear data to be used
EG(..)	- group boundaries for block 7, an input specified energy point set for block 8, and it is omitted for block 9.
WORK(..)	- working field
LFR	- length of the working field
BFG(..),BFK(..)	- buffer field for RFOD and auxiliary file, respectively
ICAT(..)	- Table of Contents for the output RFOD
JPAS(..)	- Data Headings for the output RFOD

In the followings details on each calculational block are given.

Block 1

Group constants produced: infinite diluted, group-averaged cross-sections from point-wise given nuclear data (formulae (2.1.1)).

Acceptable format types: NTF=1,6,11,21.

NTF=1 - generally, this is a simple data set produced by PRAFO
NTF=6 - this may be produced by PRAFO in the case of a very large (KEDAK)

or linearized (UKNDL) data set. Such a data set can also be produced by linearization process performed by block 8.

NTF=11 - this data format is typical for a threshold reaction.

NTF=21 - temperature dependent cross-section may be represented by this format. This type is mainly generated by block 8.

The name of the group constant (in default case) should be specified by

$$NTNAM=10000*n+NTN$$

where NTN is the data type name of the cross-section to be averaged. If n=0 then the cross-section σ if n > 0 then $(\sigma)^{-n}$ is averaged. This situation may be changed by altering the function FIQ(X) (see section 3.13)

Required input: NTNAM,

Optional input: NR(1), NR(2) first and last group to be calculated.

In the region, where the cross-sections ought to be calculated from resonance parameters and background cross-sections, the averaged cross-sections are taken to zero.

Output: the averaged cross-sections and group flux are printed and, by request, written into an SFGK file.

The required dynamic length:

IF NTF=1,11 or 21 then

$$LBL1=NDAT+(NDAT_i)_{max}+2*NGR$$

where NDAT is the number of energy points covering the energy interval in which group constants are to be calculated. $NDAT_i$ is the number of energy points covering group i. NGR is the number of groups for which constants are calculated that is NGR=NR(2)-NR(1)+1.

The case NTF=6 uses no place in the dynamic field.

Block 2

Group constants produced: Greuling-Goertzel slowing down constants from angular distribution of elastic scattering. (formulae in section 2.7). The angular distribution may be given either point-wise (NTF=21) or by Legendre expansion coefficients (NTF=11). In the energy region where the elastic scattering is isotropic the analytical formulae of constants are used. Above this region the numerical integrations are carried out by means of the numerical integration subroutine package.

Required input: NFEL=2, NTNAM (arbitrary)

Optional input: NR(1),NR(2) first and last group to be calculated ,

AM - the mass limit above which only μ and ξ are calculated. (Default: AM=28.)

Output: the Greuling-Goertzel constants are printed and, by request, are written into an SFGK file.

The required dynamic length:

$LBL2=1+NGR*NGRUL+NFN+2*MANG+5(ND_i)_{max}$

where

$NGR=NR(2)-NR(1)+1$

NGRUL=2 or 6 depending on whether A > AM or A $\leq$ AM (A is the reduced mass of scatterer)

NFN - number of angular distributions given in the file

ND_i - number of angular distribution energy values which cover the group interval

MANG - maximum number of μ values or Legendre coefficients used for the specification of angular distribution.

Block 3

Group constants produced: Inelastic scattering group transfer matrix from point-wise level excitation cross-section and/or from total inelastic cross-section.

In files the discrete level excitation cross-sections are given up to a definite energy point above which either they are taken to zero (case ENDF/B) or no more energy points are given. (case KEDAK and UKNDL). Above the region of the resolved excitation levels the inelastic slowing down matrix can be calculated only by the evaporation model from the excitation cross--section of the unresolved inelastic levels- if it is given. If not, then the total inelastic scattering cross-section is used for this purpose. In the first case the evaporation model is used from the threshold energy of unresolved levels in parallel with the calculation of inelastic scattering on resolved levels.

For level excitation cross-sections: NTF=11, for unresolved levels and total inelastic scattering cross-sections NTF=1 is accepted.

Required input: NFEL=3, NTNAM (arbitrary)

Optional input: NR(1), NR(2) first and last outscattering group to be calculated, TMAG (nuclear temperature (default:0.16)).

Output: The triangular inelastic scattering matrix and total inelastic scattering cross-section calculated from this matrix are printed and, by request are written into an SFGK file.

Required dynamical length:

$$LBL3=NGR+(NGR*(2*NGIN-IGO+1))/2+\left(NDAT^d+(NDAT_i^d)_{max},NDAT^c+3*(NDAT_i^c)\right)_{max}$$

where

$NGR=NR(2)-NR(1)+1$

NGIN=NG-NR(1)+1 - NG is the total number of groups in the group system

IGO - the group containing the threshold energy of inelastic scattering

$NDAT^d$, $NDAT^c$ are the number of energy points of resolved and unresolved (or total) inelastic cross-sctions covering the energy interval in which the constants are to be calculated

$NDAT_i^d$, $NDAT_i^c$ are the number of energy points of resolved and unresolved (or total) inelastic cross-section covering the group i.

Block 4

Group constants produced: infinite diluted and self-shielded temperature dependent group averaged constants for the total, (n,γ), elastic, and fission cross-sections, respectively. The basic fomulae are presented in section 2.1. This task is performed in the whole energy region disregarding whether the cross-sections are specified by point-wise or by resonance parameters.

Point-wise region: The total cross-section may have a format type NTF=1,6, or 21. The format type NTF of other data should be the same as that of the total cross-section or zero, otherwise an error message is generated and the calculation will not be performed. Any of the (n,γ), elastic and fission cross-sections may be changed to another type of cross--section overriding the default data type request from input (see section 3.7).

Resolved resonance region: the resolved resonance parameters may be either single or multilevel ones. The two cases are distinguished by the control parameter EFLAG(1). The lower and the upper boundary of the resolved resonance region are specified by EL(1) and EU(1), respectively.

Unresolved resonance region: the formalism prescribed for this region for KEDAK data somewhat differs from that prescribed for ENDF/B data. The two cases are distinguished by the control parameter EFLAG(2). The lower and the upper boundary of the unresolved resonance region are specified by EL(2), and EU(2), respectively.

EL, EU and EFLAG are RFOD data (NTN=4511) but they may be overriden by input. EFLAG also controls whether or not a background cross-section should be added to the cross-section calculated from the resonance parameters. The possible values of EFLAG are shown in the table below.

EFLAG(1)

1,11	single-level Breit-Wigner parameters
2,12	multi-level Breit-Wigner parameters

EFLAG(2)

1,11	without overlapping correction and without energy dependence of average level density $\bar{D}$ (ENDF/B)

2,12 without overlapping and with energy dependence of average level density $\bar{D}$

3,13 with overlapping correction and energy dependence of average level density $\bar{D}$ (KEDAK)

4,14 with overlapping correction and without energy dependence of average level density $\bar{D}$

If EFLAG < 10 no background cross-section should be added
If EFLAG > 10 background cross-section should be added

Input required: NFEL=4, NTNAM (arbitrary)

Optional input: first and last group to be calculated: NR(1) NR(2); accuracy parameters for integration: NUJM, ERR, M, EZ, SMIN, NRES, NLETH.

Output: printed output contains the infinite diluted total and the three other cross-sections, temperature and σ values, the corresponding self-shielded cross-sections, f-factors and fluxes. On request all these quantities (except the f-factors) can be written into an SFGK files

In the resolved region the accuracy of integration is governed by NUJM and ERR. If NUJM > 2 then the integration between the peaks is performed by Romberg's method with accuracy ERR. If NUJM=1 then the group interval is divided into sub-intervals equidistant in lethergy of width ΔU=ERR and the integral is calculated as the sum of $f(E_k)*\Delta U$ where E_k is the middle of sub-interval k.

In the unresolved region the group interval is divided into NLETH parts. equidistant in lethargy and the unresolved resonance cross-sections are calculated for the middle point of each interval.

The calculation of group averaged total cross-section in the resolved and unresolved range regions differs. In the unresolved region the self-shielded total cross-sections by points are calculated first and then the averaging of the inverse is performed. In the resolved region the inverse total cross-sections are averaged. This may give rise to an incorrect value of self-shielded total cross-section for the group into which the meeting point of the two regions falls. In this case, if the self-shielded total cross-section is important, a change of in region boundary is recommended.

Before calling block 4 the parameter specification, controlled by namelist card TSGO is compulsory.

Required dynamic length:

LBL4=2+NT+NSI+NGR*(7+5*NT*NSI)+MAX(LHP,LHRR,LHUR)

where

LHP is the dynamic length in the case of point-wise data. If NTF=1 or 21 then LHP=4*NDAT is the number of energy points for the total cross-section covering the energy intervals in which group constants are to be calculated.

If NTF=6 then
LHP=NT*NSI+2*(NTT+NT+2) where NTT+1 is the length of a sub-set of data.
NT - number of temperature values
NSI - number of σ_o values
NGR - number of groups to be calculated
LHRR is the required dynamic length in resolved resonance region
LHRR=13*JR+4*NDAT+MAX(NDAT,$(LPN)_{max}$+42*NSI+7+NUJM*6*NSI) where NDAT is the number of energy points for the total background cross-section covering the energy intervals in which the group constants are to be calculated, JR is the number of resolved resonance sets, LPN_i=3* (number of resonance peaks in group i), NUJM is the number of bisections of the integration interval (see 2.4) and LHUR is the required dynamic length in the unresolved resonance region:
For KEDAK data
LHUR=NLETH+1+(17*NE)*ND3+4*NT*NSI
and for ENDF/B data
LHUR=5*(NLETH+1)+20+(4*NT*NSI+4)*(NLETH+1)
NLETH is the number of lethargy subinterval specified for the calculated energy interval
ND3 is the number of resonance series
NE is the number of energy points covering the given energy interval and for which unresolved resonance parameter sets are specified.

Block 5

This is a user specified free block. On the formal parameter list there is only one data heading.

Block 6

Group constants produced: Legendre momenta of elastic scattering transfer matrix (up to 5). Point-wise elastic scattering cross-section and the quantity $\pi_\ell(E\to i)$ defined in 2.6 are used. The RFOD to be used by this block cannot be a PRAFO made one but it is a product of blocks 7 and 8 or 9.

Input required: NFEL = 6, NTNAM (arbitrary), NR(1), NR(2) the first and last group to be calculated. One should take care that the energy interval specified for $\pi_\ell(E\to i)$ covers the energy range of the required groups. Other wise we get wrong results without any error message.

Output: the elements of the momenta of elastic scattering matrix are printed and, by request, are written into an SFGK file.

Required dynamic length:
LBL6=MAX(2*NDAT,NGR*IMAX*NM1+2*$(NDAT_i)_{max}$+2*(NLETH+1+NC))

where

NDAT is the number of energy points for elastic scattering cross-section covering the energy interval to be calculated

NGR=NR(2)-NR(1)+1

IMAX is the maximum number of inscatter groups for one outscatter group

NM1 is the number of momenta

$NDAT_i$ is the number of energy points for elastic scattering covering the group i

NLETH number of sub-intervals (see Block 7)

NC is the number of elastic angular distributions in the energy interval to be calculated.

Block 7

Data produced: Legendre momenta of elastic transfer probabilities from energy points to groups, $\pi_\ell(E\to i)$ (see section 2.6). The outgoing nuclear data is the angular distribution of elastic scattering which may be given either point-wise or by Legendre expansion coeffecients.

The energy mesh for $\pi_\ell(E\to i)$ is specified in the following way:

Let E1 < E2 be the boundaries of an inscattering group, and EMAX the maximal energy change by collision. If E1+EMAX < E2 then the interval between E1 and E1+EMAX is divided, equidistant in lethargy, into NLETH parts. Between E1+EMAX and E2 those and only those energy points are taken at which angular distribution is specified. If E1+EMAX$\geq$E2 then the interval between E1 and E2 is divided, equidistant in lethargy, into NLETH parts. The interval between E2 and E2+EMAX is also divided, equidistant in lethargy, into NLETH parts. The energy point set generated in this way is joined with the energy points of elastic scattering cross-section and the integration is performed on the resulting energy mesh by the block 6.

Input required: NFEL=7, NTNAM=2002, NT - is the number of momenta, NR(1), NR(2) the first and last inscattering group. If $\pi_\ell(E\to i)$ are to be used in block 6 then the specified inscattering groups should contain all possible inscattering groups corresponding to the outscattering groups specified for block 6.

The output of the results is in RFOD form, which can be printed out by request (see. 3.7).

Required dynamic length:

LBL7=(NLETH+1+NC)*(2+NT)+6*MANG

where

NC is the number of elastic angular distributions in the energy interval of calculation

MANG is the maximum number of values or Legendre coefficients used to specify angular distribution.

Block 8

Data produced:

a/ point-wise cross-sections for a user-specified energy point set from any point-wise cross-section set,

b/ Doppler-broadening of a linearly interpolable point-wise cross-section set (energy points are unchanged)

c/ Linearization of a non-linearly interpolable cross-section set.

In case a/ the NTF of the input set may be 1 or 6, the NTF of output set is always 1.

In case b/ the NTF of input set may also be 1 or 6, the NTF of the output set is 21 if that for the input set is 1, and 6 if it is 6. For NTF=1, the subroutine BROADN (taken from the code package AMPX [18]) is used for numerical Doppler broadening, for NTF=6 this is performed by DOPSIL made available by B. Bohmer (ZfK, Rossendorf, GDR)

In case c/ the NTF of the input set is always 1 and that for the output set is always 6.

Input required: NFEL=8, NTNAM (=NTN the output data will have this type name), NG=0 in case b/, NG=-1 in case c/, ER(1), ER(2) - lower and upper bounds, respectively of the energy interval for which the point-wise cross-sections are required.

The output of the results in RFOD form, which can be printed out by request (see section 3.7).

Required dynamic length:

If the input NTF=1 then LBL8=3*NDAT

where NDAT is the number of energy points covering the energy interval ER(1), ER(2)

If the input NTF=6 then for a/ no further dynamic space is required; for b/ all available space may be required. Here, as the Doppler broadening calculation requires an energy point set extended to a large energy region the accuracy of calculation may depend on the available free dynamic space.

Block 9

Data produced: temperature dependent total, (n,γ), elastic and fission point-wise cross-sections from pointwise cross-section, resolved resonance parameters and unresolved resonance parameters. In the unresolved resonance region the self-shielded cross-section values can also be calculated.

Point-wise region: the total cross-section may have a format type NTF=1 or 21. The format type of other data should be the same as that of the total cross-section, or zero; otherwise an error message is generated and the calculation will not be performed. Any of (n,γ), elastic and fission cross-sections may be changed to an other type of cross-section by overriding the

default data type request from input (see 3.7).

The control of the calculation in the resolved and unresolved resonance regions is the same as for block 4.

The NTF of the output data is 7 or 8. The latter is used when a resonance shielded cross-section is required in the unresolved region. The energy point set is specified in the following way:

- for a point-wise region: the original set is retained
- for resolved resonance region in the following may. If NUJM=1 then we get a lethargy mesh ERR. If NUJM $\geq$ 2 then the required energy interval is divided into sub-interval in such manner as is done in the case of group constant calculation. (see block 4). Within a sub-interval the points are taken as dense as sufficient for linear interpolation (with given accuracy) of cross-section set.
- for unresolved parameters: the specified energy interval is divided, equidistant in lethargy, into NLETH parts.

Input required: NFEL=9 NTNAM (arbitrary, the output data will have this type name), ER(1), ER(2) - lower and upper bound of energy interval for which the point-wise cross-sections are required.

The output of the results is given in RFOD form, which can be printed out by request, (see section 3.7).

Before calling the block 9 the parameter specification controlled by namelist card TSGO is compulsory. If NSI > 0 is specified on this card then only that part of specified energy region is calculated which is contained by the unresolved resonance region.

Required dynamic length:

LBL9=MAX(LHP,LHRR,LHUR)

where

LHP is the dynamic length in the case of point-wise data. LHP=4*NDAT, where NDAT represent the energy points for the total cross-section covering the specified energy intervals LHRR is the required dynamic length in resolved resonance region LHRR is the required dynamic length in resolved resonance region

$$LHRR=13*JR+5NDAT+(LPN)_{i,max}+4*NT+LRMAX$$

where JR is the number of resolved resonance sets, NDAT is the number of energy points for the total background cross-section covering the specified energy interval, LPN=3*(number of resonance peaks in the specified energy interval), LRMAX is the maximum number of points within a sub-interval. Practically, it is impossible to estimate it correctly. (It can only be highly overestimated) Accordingly, a suitable guard against field overflow is built in.

LHUR is the required dynamic length in the unresolved resonance region. It is exactly the same as that for block 4 and is thus not given here.

Block 10

This is a user specified free block for point-wise cross-section manipulation. On the formal parameter list there is only one data heading.

3.7 THE WORK OF THE NWZ-3 PROGRAM INPUT DESCRIPTION

The NWZ-3 program is controlled by six control modules each of which is called from the main control segment. In the following table these are listed in calling sequence.

Module	Description
CTRLF3	specifies the output level, identification number and RFOD and SFGK files to be used
PARMIN *	specifies the auxiliary parameters (T and σ_o)
GRPSF3 **	specifies the group system
FLUXF3 **	specifies the averaging spectrum
MTBPF3	specifies the material to be calculated
CALCF3 ***	specifies the type of group constants and related quantities, controls the calculation with blocks

* Requested only for blocks 4, 8 and 9
** The call of these can be interchanged whith each other
*** It contains a cycle by calculational blocks which may be interrupted by control input (see below)

In the following tables the namelist input cards are described which at the same time control the calling of the modules. The namelist cards, except for modules CTRLF3 and MTBPF3, can be followed by free format input. (A flow chart is given in Fig. 2)

CTRLF3 namelist name: CTRL

Var. name	Default	common name pos.	Description
NOUT	6	PEIF 2	log. number for printed output
NLIB	2	PEIF 3	log. number for RFOD
NGL	0	PEIF 4	log. number for unformatted SFGK
MGL	0	PEIF 5	log. number of formatted SFGK

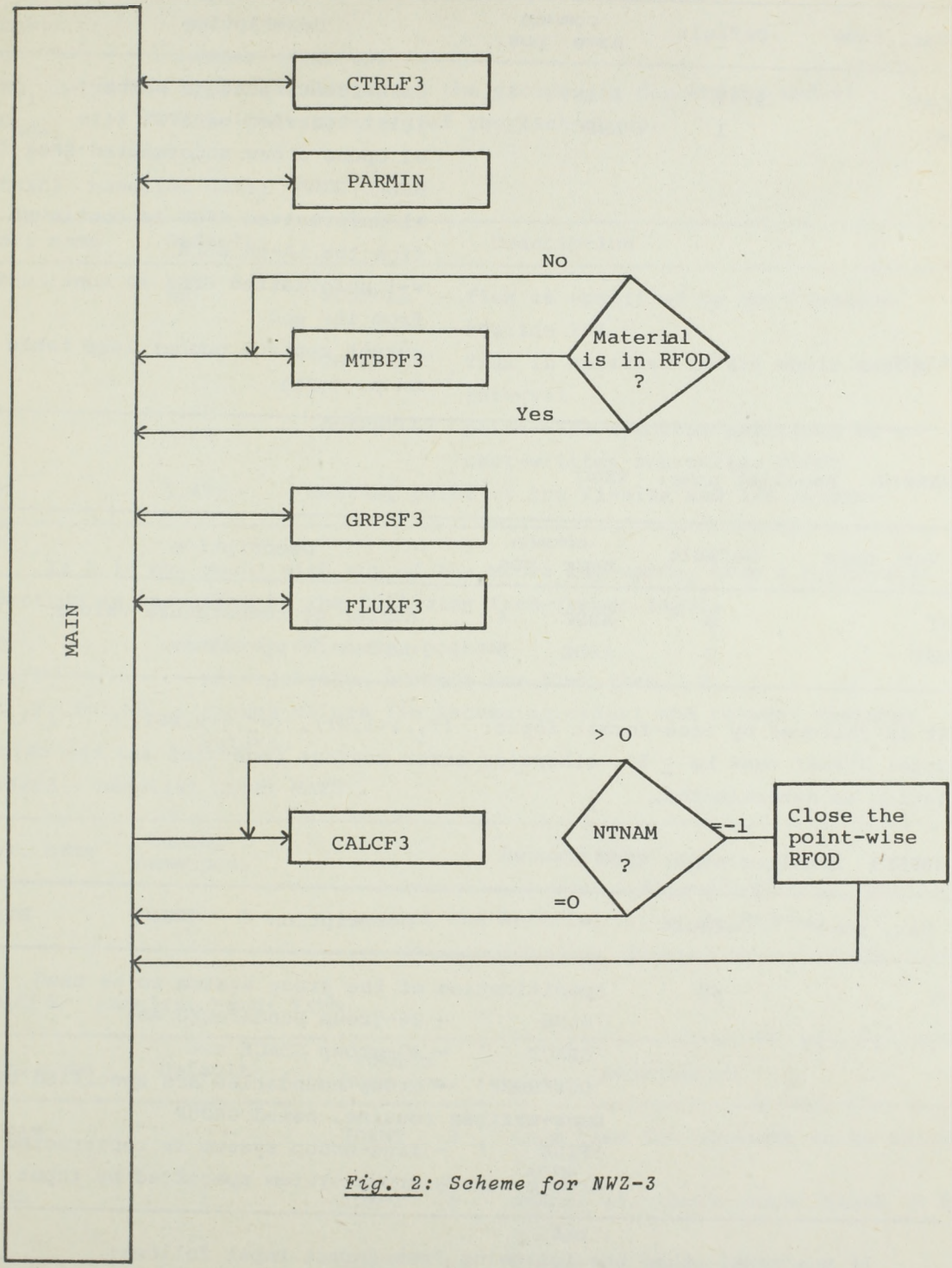


Fig. 2: Scheme for NWZ-3

Var. name	Default	common name	pos.	Description
KDAT	9999	IDENT	4	task identification number
LA	1	ABSC	3	initialization of SFGK file =1 opens a new unformatted SFGK (if NGL≠0) >1 unformatted SFGK is continued from the LA-th word =-1 unformatted SFGK is continued from its end
NCOUT	0			output control number (see table on p. 3.25)

PARMIN namelist name: TSGO

Var. name	Default	common name	pos.	Description
NT	0	ABSC	4	number of temperature values
NSI	0	ABSC	5	number of σ_o values

It is followed by free-format input: $(T_i, i=1,NT)$, $(\sigma_o^j, j=1,NSI)$
Note: NT+NSI must be $\leq$ 50, otherwise error message generated and the calculation is determinated.

GRPSF3 namelist name: GROU

Var. name	Default	Description
X	8H	specification of the group system to be used 'BANB ' - 26-group Bondarenko set 'GRACE ' - 40-group GRACE set 'OUTERGRP' - group boundaries are specified by a user-written routine, named GROUP 'FINE ' - fine-group system is constructed from a course group system specified by input

If x ='FINE' then the following free-format input follows:
NI - number of coarse gorups
$(EP_i, EM_i, MK_i, JI_i, i=1,NI)$ - upper and lower boundaries of coarse groups, number of fine groups in given course group, if JI>0, the division is uniform in energy, if JI>0, the division is uniform in lethargy.

If X is not equal with any of the above key-words, then the group boundaries are to be specified by the following free-format input:

NG - number of groups

$(EG_i, i=1,NG)$ - upper boundaries of the groups (in descending order)

EG_{NG+1} - the lower boundary of the last group.

FLUXF3 namelist name: SPEC

Var. name	Default	Description
X	8H	'FORMULA' - flux is specified by the function routine PHI
		'CONSTANT' flux is constant in the whole energy interval
		'OUTERFLU' point-wise spectrum specified by a user-written subroutine FLOUT
PK	1.4E6	meeting point of the fission and 1/E spectra

If X is not equal with any of the above key-words, then a point-wise spectrum is specified by the following free-format input:

NP - number of energy points

IA,IF - interpolation numbers for flux (see 3.9)

$(E_i, F_i, i=1,NP)$ - energy values (in ascending order) and related spectrum values.

MTBPF3 namelist name: MATE

Var. name	common name pos.	Description
MATN	IDENT 1	name of the material to be calculated

CALCF3 namelist name: TYPE

Var. name	Default	common name pos.	Description
NTNAM		IDENT 2	type name for constant to be calculated
NFEL	1	IDENT 3	number of calculational block to be called
NT*		ABSC 4	number of Legendre moment
NSI****		ABSC 5	number of σ_o' is
NR(2)	1,NG	IDENT 5,6	first and last group to be calculated
AM	28.	DOPT 3	mass limit for Greuling-Goertzel constants

Var. name	Default	common name	common pos.	Description
ER(2)	0.,2.5E7	ADJB6	5,6	energy interval for point-wise cross-sections to be calculated
NAUX	9	NAUXF	1	log. number for an auxiliary scratch file.
NPOINT	8			log. number for the point-wise RFOD to be produced
NREQ**	0			number of required types, if NREQ = 0 then the default requirement is valid
LRF1	40			length of ToC for point-wise RFOD to be produced
LRF2	140			length of DHs for point-wise RFOD to be produced
NUJM	10	ACCU	1	division limit for integration or linearization
ERR	0.01	ACCU	2	accuracy limit for integration or linearization
NLETH	10	ADJB6	7	number of lethargy intervals for unresolved resonance or scattering matrix calculation
AW		MTDAT	1	values corresponding to the
Z		MTDAT	2	values given in RFOD under the
RIS		MTDAT	3	type name 458***
RLAM		MTDAT	4	values corresponding to the
RR		MTDAT	5	values given in RFOD under the
EB		MTDAT	6	type name 459***
EL(2)		MDAT	7,8	values corresponding to the
EU(2)		MTDAT	9,10	values given in RFOD under the
EFLAG(2)		MTDAT	11,12	type name 4511***
NG	def.in GRPSF3	DOPT	2	number of group (required for block 8)
M	2	ADJB6	1	number of exactly calculated neighbouring resonances
EZ	100	ADJB6	2	interval (in half-width) for Doppler calculation
SMIN	0,1	ADJB6	3	minimum value for resonance scattering cross-section
NRES	10	ADJB6	4	number of resonances to be taken into account on both sides of an energy point.

* It is used for block 7

** The NREQ names of required types follow the namelist card TYPE in free-format. The order of these types is given for each block in the table below.

*** Required, if there is no such type on the input RFOD.

**** This is used in the case of block 9 when only unshielded cross-sections are required in the unresolved range.

Note: The namelist card after a namelist card TYPE should also be a card TYPE unless NTNAM $\leq$ 0.

If NTNAM=0 then the control is returned to the main program

If NTNAM=-1 then the compilation of point-wise RFOD will be finished and the control returned to the main program.

Order of required types/block

block	NREQ	Description of required types
1	1	data type name of point-wise cross-section on RFOD
2	1	data type name of angular distribution for elastic scattering
3	3	-data type name of discrete inelastic level cross-sections (NTF=11) -data type name of total inelastic scattering cross-section (NTF=1) -data type name of cross-section for unresolved inelastic scattering levels (NTF=1)
4	7	-data type name of total background cross-section -data type name of elastic background cross-section -data type name of (n,γ) background cross-section -data type name of fission background cross-section -data type name of resolved resonance parameters -data type name of energy independent unresolved resonance parameters -data type name of energy dependent unresolved resonance parameters
6	2	-type name assigned to inscattering probabilities produced by block 7 -type name of elastic scattering cross-section produced by block 8
7	1	the same as for block 2
8	1	the same as for block 1
9	7	the same as for block 4

Note: The default data type requirements for blocks are in accordance with those given in 3.3

Output control number: NCOUT=ΣNK

NK	Output performed (on log. numb NOUT=6
1	all input namelist cards
2	output of the group boundaries
4	output of the averaging flux
4	print the whole RFOD produced by blocks 7-10
8	print data types available on RFOD
16	output of messages on the convergence of resonance calculation

3.8 STRUCTURE OF SFGK FILE

An SFGK file consists of a series of SFGK sets. Before each SFGK set a word 'BEGN' appears and the word 'END' closes the SFGK file.

An SFGK set consists of 7 integers and real numbers. The 7 integers are as follow:

MATN - material name
NTNAM - constant type name
NFEL - number of processing block
KDAT - task identification number
NR1,NR2 - first and last processed groups
NL - is the length of the real part of the SFGK set

The structure of the real part depends on the processing block is described in the following.

Block 1

NL=2*NG

$(\langle\sigma_x\rangle_\infty^i,\ i=NR1,NR2),(\phi_i,\ i=NR1,NR2)$

$\langle\sigma_x\rangle_\infty^i$ - group averaged infinite diluted cross-section of reaction x

ϕ_i - group averaged flux

Block 2

NL=2*NG+1 or 6*NG+1 depending on the atomic mass A

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

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

The quantities in [...] are given when A $\leq$ AM, where AM is a mass limit to be specified by input (default 28.0)

Block 3

NL=(IGS-NR1+)*(1+(2*NGO-NR1+IGS+2)/2)+1

$(\langle\sigma_{in}\rangle^{i},\ i = NR1,NR2)((\langle\sigma_{in}^{i\to}\rangle^{j},\ j=i,NGO),\ i=NR1,IGS),\ RIGO$

where

IGO is the group containing the threshold energy of inelastic scattering, RIGO=IGO+0.01, IGS=MINO(IGO,NR2)

Block 4

NL=2+NT+NSI+(6+5*NSI*NT)*NG

$NT,NSI,(T_i,i=1,NT),(\sigma_o^i,i=1,NSI),(\langle\sigma_t\rangle_\infty^i,\ i=NR1,NR2),$

$(\langle\sigma_\gamma\rangle_\infty^i,i=NR1,NR2),(\langle\sigma_s\rangle_\infty^i,i=NR1,NR2),(\langle\sigma_f\rangle_\infty^i,i=NR1,NR2),i=NR1,NR2),$

$(((\langle\sigma_t(T_k,\sigma_o^j)\rangle^i,\ \langle\sigma(T_k,\sigma_o^j)\rangle^i,\ \langle\sigma_s(T_k,\sigma_o^j)\rangle^i\ k=1,NT),j=1,NSI),i=NR1,NR2),$

$(((\emptyset_i(T_k,\sigma_o^j)^i,\ k=1,NT),j=1,NSI),I=NR1,NR2),(\emptyset_i,i=NR1,NR2)$

where

NT - number of temperature values, T_i - temperature values
NSI - number of σ_o values, σ_o^j - values
NR1,NR2 - first and last group to be calculated

$\langle\sigma_t\rangle_\infty$, $\langle\sigma_\gamma\rangle_\infty$, $\langle\sigma_s\rangle_\infty$, $\langle\sigma_f\rangle_\infty$ total, (n,γ), elastic scattering and fission group averaged infinite diluted cross-sections, respectively and

$\langle\sigma_t(T_k,\sigma_o^j)\rangle$, $\langle\sigma_\gamma(T_k,\sigma_o^j)\rangle$, $\langle\sigma_s(T_k,\sigma_o^j)\rangle$ and $\langle\sigma_f(T_k,\sigma_o^j)\rangle$ group averaged, self-shielded total, (n,γ), elastic scattering and fission cross-sections, respectively. $\emptyset(T_k,\sigma_o^j)$ and ∅ self-shielded and infinite diluted group averaged flux, respectively.

Block 6

$$NL=2+NG+(M+1)*\sum_{i=1}^{NG} IMAX_i$$

$O,M,(IMAX_i+0.01,((\sigma_m^{i\to i+k-1},\ m=0,M),\ k=1,IMAX_i),\ i=NR1,NR2)$

where

M - highest Legendre momentum
$IMAX_i$ - number of possible inscatterings for a scattering in group i,
NR1,NR2 - first and last group to be calculated
NG=NR2-NR1+1

A card-image form, for transmission purposes, is defined for the SFGK sets. This is given in the following Table.

Card	FORMAT	Content
1	6I12	MATN,NTNAM,NFEL,KDAT,NR1,NR2
2	I12	NL - length of real part
3 etc	6E12.5	real part, that is the constants

These sets can appear on the output of log. number NPUN.

3.9 SUBROUTINE PACKAGE FOR NUMERICAL INTEGRATION

The FEDGROUP numerical integration package consists of the following subroutines:

FXINT,ESINT,SINT,CRINT,PHINT,PHINF,FINT,ZWIN

SUBROUTINE ZWIN(NDAT,EP,EM,E,I1,I2)

Input parameters:

E(..) - energy values in ascending order
EP≥EM - energy interval
NDAT - number of energy points

Output parameters:
integers I1,I2 for which
$E(I1) \leq EM < E(I1+1)$ and $E(I2-1) \leq EP < E(I2)$

An improved version of ZWIN prepared by A. Trkov (Institut Jozef Stefan, Ljubljana, Yugoslavia) is used in FEDGROUP-3

SUBROUTINE FINT(SG2,SG1,E2,E1,E,IA,IF)

general interpolation routine, where (E1,SG1),(E2,SG2) and (E,FINT) are the two end points and the interpolated point, respectively.

IA and IF are interpolation numbers which are in close relation with that of ENDF/B [4] and are given in the following table:

IA	IF	ENDF/B	Definition
1	1	2	SG is linear in E
2	1	3	SG is linear in log(E)
1	2	4	log(SG) is linear in E
2	2	5	log(SG) is linear in log(E)

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

This is defined as

$$CRINT = \int_{EM}^{EP} FUN(E,APAR,LPAR)dE$$

The integral is calculated by Romberg's procedure, The maximum number of points is 2**NUJM+1, where NUJM is specified by input (default value 10), but it cannot be more than 20. APAR(..) is a parameter set, LPAR may be the length of it or may be any other integer parameter.

FUNCTION PHINF(E,APAR,LPAR) and FUNCTION PHINT(E,APAR,LPAR)

PHINF and PHINT give the product flux and cross-section at the energy point E, for formula given and point-wise given flux, respectively. The cross-section and flux points are given through the parameter field APAR.

FUNCTION FXINT(EP,EM,SGN,ES,FL,EF,NSP,NDAT,IA,IF)

This is defined as

$$FXINT = \int_{EM}^{EP} dE\ SGN(E)*FL(E)$$

FUNCTION ESINT(ES,SGN,EF,I1,I2,IA,IF)

This is defined as

$$ESINT = \int_{ES(I1)}^{ES(I2)} dE\ SGN(E)*FL(E)$$

FUNCTION SINT(SG1,SG2,E1,E2,IA,IF,EF,FL,NSP)

This is defined as

$$SINT = \int_{E1}^{E2} dE\ FINT(SG2,SG1,E2,E1,E,IA,IF)*FL(E)$$

For these last three subroutines the meaning of the notation is:

ES(..),SGN(...) - energy points and cross-sections
EF(..),FL(..) - energy points an flux values
NDAT - number of cross-section points
NSP - number of spectrum points

3.10 EVDAUT PROGRAM FOR HANDLING DATA IN CARD-IMAGE FORMAT

Because of the incompatibility of PL/1 and FORTRAN, this program should be used in a separate job step.
The program performs the following functions:
- copying a selected part of the card-image file
- printing selected records

- during copying it changes characters, adds (deletes) cards to (from) the output file.

The DDNAME used:

INTAP - data file to be copied

OUTAP - resulting file

The work of EVDAUT is controlled by data-directed input cards, whose parameters are presented in the following table whose.

Var. name	Default	Description
TASK	0	control number of the function to be performed =0 file segment copied =1 file segment copied and selected records will be printed =2 selected records from a file segment will be copied =3 the copied file segment should be changed
N1	0	the file segment begins from the N1+1-th record
N2	999999	the file segment ends with the N2-th record
PATRN		records with this string will be selected
CHAR		the PATRN string should begin from the CHAR-th character of the selected records
TAPE	'CCCCCC'	this string of 6 characters printed after each printed record
CHLEN		length of the string PATRN

In the case of TASK=3 control data for changes to be performed are required. These data are given by list-directed input right after the related data--directed control card. The data items are:

1. the place of the first character of the identifying string on the card to be chosen for changing operation
2. length of the identifying string
3. identifying string
4. correction string replacing the identifying string
5. control integer, if this <0, then cards, whose number equals the absolute value, will be omitted from the file, beginning from the identified card; if this $\geq$ 0 then the identified card is corrected and cards, whose number equals the control number, are inserted.

EVDAUT is terminated if the end-of-file is reached either on INTAP or on SYSIN. In the case of tape error, an error massage is generated and the processing continuous.

3.11 RFODS PROGRAM FOR MANIPULATION WITH RFOD FILES

The control module of the RFODS program is called from the main control module by giving the namelist card RFOD.

The possible program's functions are the following:

- print the content of the RFOD file ('PRINT')
- merge the whole RFOD file ('ALL') with that of the file to be compiled
- merge selected data sets from an RFOD file with all data sets of those to be compiled ('INCL' or 'EXCL')
- merge data set with $6 \leq NTF \leq 8$ ('UNIF')

The strings in parenthesis are the key-words for manipulation. There are two other key-words, viz:

'BEGN' - the beginning of the compilation of the new RFOD

'FINS' - the end of the compilation of the new RFOD

The input for RFODS the program is given in the table below:

Namelist name: RFOD

Var. name	Default	Description
XMOD		key-word for manipulation
NLIB	2	log. number of input/output RFOD*
NGL	8	log. number of the auxiliary file
NOUT	6	log. number for printed output
NCOUT	0	output control number
LC	900	buffer length
LK	18	length of the comment of the RFOD to be compiled
NMAT	1	number of materials to be copied
LRF1	100	estimated length of ToC of RFOD to be compiled
LRF2	500	estimated length of DHs of RFOD to be compiled

After the namelist card, depending on XMOD, further input may be required:

XMOD='BEGN' N=(LK-1)/18+1 comment cards

XMOD='EXCL' 'INCL' free-format cards containing the names of materials and types to be excluded/included from the input RFOD by performing the merging operation for one material the following are inputed:

MATN - material name

NTYP - number of types

$(NTN_i, i=1,NTYP)$ - names of type

In the case of 'UNIF' the data sets with $6 \leq NTF \leq 8$ are merged in sequence of descending type names. The resulting RFOD will be in the place of the old one.

*NLIB becomes output RFOD after XMOD='FINS', otherwise it is input RFOD.
NB. If the NLIB value is not changed by the card containing XMOD='FINS', the last input RFOD will be overwritten!

Output control number: NCOUT=Σ NK

NK	Output performed
1	print the input namelist card
4	print the whole RFOD file
16	print the first and the last data point

3.12 SFGKS PROGRAM FOR MANIPULATION WITH SFGK FILES

The control module of the SFGKS program is called from the main control module by giving the namelist card SFGK.

The possible program's functions are the following:

- print out a table of content of SFGK ('EXPLORE')
- copy of selected sets ('COPYSELE')
- copy of the whole SFGK except certain sets ('COPYEXCL')
- merging SFGK sets containing the group constants for the same elements, type and group system but for different groups ('COMPLETE')
- copy the SFGK sets and change KDAT to a specified value ('CHANGE')

The strings in parantheses are the key-words for manipulation. A key--word 'FINISH' terminates the SFGK manipulations.

The input of the SFGKS program is given in the following table

Namelist name: SFGK

Var. name	Default	Description
FUNC		key-word for manipulation
NOUT	6	log. number of printed output
NPUN	0	log. number for formatted SFGK
NGK1	3	log. number for input SFGK
NGK2	2	log. number for output SFGK
LC	900	buffer length
ID(6)	0	integer part of an SFGK set to be retrieved*
LA	1	initialization of SFGK file =1 open a new unformatted SFGK (if NGK2≠0) >1 unformatted SFGK is continued from the LA-th word =-1 unformatted SFGK is continued from its end
LMAX	3000	the estimated length of the longest SFGK set

Var. name	Default	Description
EPS	0.01	error of parameters
NG		number of groups (required for 'COMPLETE' function)
KDATN		new KDAT (required for 'CHANGE' function)
NCOUT	0	output control number

* For identification only the non-zero elements of input specified ID are taken into account. This facilitates the retrieving the group of data sets by one control card.

If group constants produced by block 4 are to be merged by manipulation 'COMPLETE', then, before calling SFGKS, the parameters T and σ_o should be specified by PARMIN, i.e. namelist name TSGO and free-format input should be used. (see 3.7) Then those group contants for which the temperature and σ_o values differ with a relative deviation less than EPS, will be selected.

Output control number: NCOUT=Σ NK

NK	Output performed
1	print the input namelist card
2	print the retrieved SFGK set(s)
4	print the SFGK sets written to the new SFGK file
8	print the merged SFGK sets

3.13 SUBROUTINES WHICH MAY BE REDEFINED BY USERS

SUBROUTINE GROUT (EG,NG)
EG(..) - group boundaries
NG - number of groups
Default: dummy
Purpose: user can define the group system in his own way. For example, read in from magnetic tape, generating with formula etc.

SUBROUTINE FLOUT (A,N)
A(1)....A(N) - energy values
A(N+1),...A(2*N) - spectrum values
Default: dummy
Purpose: user can define the averaging spectrum in his own way. For example, read in from magnetic tape, generating with formula etc.

FUNCTION PHI(E)
E - energy, PHI - spectrum value

Default

$$PHI = \begin{cases} C*EXP(-E_m/0.965)*(EXP(\sqrt{2.29E_m})-EXP(-\sqrt{2.29E_m}))/2 & \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{if } E > PK \\ 1/E \qquad\qquad\qquad\qquad\qquad \text{if } E \leq PK \end{cases}$$

E_m is E in Mev, C ensures the continuity of the spectrum at E = PK; PK is to be specified by input (default 1.4E6)

SUBROUTINE SOKPR(ICAT,IPAS,PAS,BFK,WORK,IWORK,LFR)
ICAT(..) - ToC of RFOD to be compiled
IPAS(..),PAS(..) - DHs part of the RFOD to be compiled
BFG(..) - buffer for RFOD
BFK(..) - buffer for auxiliary file
WORK(..),IWORK(..) - dynamic field
LFR - length of the dynamic field

The length of ToC (LHCT), DH parts (LPAS) and data parts (LDAT) are given over the COMMON/WBND/ in position 5,4, and 3, respectively.

Default: dummy.
Purpose: user may place his own PRAFO in the system through this subroutine.

SUBROUTINE F3BLO5(IPAS,EG,EF,FL,WORK,LFR,BFG,BFK)
IPAS(..) - data heading(s) of the data used in this block
EG(..) - group boundaries
EF(..),FL(..) - averaging spectrum energy and values
WORK(..) - dynamic field
LFR - length of the dynamic field
BFG(..) - buffer for RFOD
BFK(..) - buffer for SFGK

Default: dummy
Purpose: user may place his own group constant calculational block into the system through this routine. Some important parameters are given over to calculational blocks through COMMONs. These are presented in the input tables of 3.7

SUBROUTINE F3BL1O(IPAS,EG,BFG,BFK,WORK,LFR,ICAT,JPAS)
IPAS(..) - data headings of the data used in this block
EG(..) - group boundaries or any set of energy points
BFG(..) - buffer of RFOD
BFK(..) - buffer for auxiliary file
WORK(..) - dynamic field
LFR - length of dynamic field

ICAT(..) - ToC of the compiled RFOD
JPAS(..) - data headings of the compiled RFOD

Default: dummy
Purpose: user may place his own point-wise calculational block into the system through this subroutine.

Except for the common variables presented in the tables of Section 3.7, the length of the data heading part (LPAS) and the length of the data part (LDAT) are given to COMMON/WBND/ in positions 9 and 10, respectively.

FUNCTION FIQ(X)
FIQ=F(X)

Default: F(X)=X if N=0, F(X)=1/(X**N) if N > 0 where N is given over through COMMON/INTG/ in the first position.
Purpose: any integration which occurs through the integration subroutine package, is, in fact, an integral

$$\int dE\ F(\sigma)*\emptyset(E)$$

The user can perform the integration of any function of cross-section by an appropriate choice of FIQ.

SUBROUTINE VIFORM(A,ID,BF)
A(..) - real numbers of a SFGK set
ID(..) - integers of a SFGK set
BFG(..) - buffer for SFGK file

Default: dummy

The user can transform the calculated SFGK set before output making use of this subroutine

3.14 JOB CONTROL PROCEDURES

A FEDGROUP job may be composed of the following steps

1 Preparation of input files.

If the input file is a card-image evaluated data file then its segment to be used in PRAFO calculation is copied to a scratch file. It is recommended that the EVDAUT program be used for this purpose. If the input is an RFOD or SFGK on magnetic tape, it is recommended that it be copied to a scratch disc file by a system utility e.g. by IEBGENER. IF RFOD or SFGK is a disc file then this step may be omitted.

2 Preparation of FEDGROUP load module. In order to be able to change the length of the dynamic field or substitute any of subroutines there is a group of job steps which prepares, compiles and link-edits the FEDGROUP program using, of course, a library and a file containing the overlay control cards.

If no change is necessary then this group of steps may be omitted and an earlier prepared load module is to be used in the following go-step.
3 Go-step: complete run of the FEDGROUP system containing all FORTRAN modules.
Various procedures can be constructed from the combination of these three steps.

3.15 ERRORS AND MESSAGES

1. Checking the required length of the dynamic field.

The one of the most frequent errors leading to the failure of a FEDGROUP run is the overflow of the dynamic field. In the most crucial places of the system the required dynamic field length is checked against the available one. If overflow occurs an arror message like

REQUIRED LENGTH n AT DISPOSAL m

is generated and the calculation is terminated.

There is no overall checking of the dynamic length, therefore an overflow may give rise to an operational system error or, in some cases, time overflow.

2. Checking the length of ToC and DHs in RFOD compilation time

If the length of the ToC or DHs becomes greater than the specified ones then an error message

PLACE FOR CATALOG OR DATA HEADING IS NOT ENOUGH i,j,k,l is

generated where i,k are the specified ToC and DHs lengths, j,l are the required ones.

There is no overall checking, especially in the case of point-wise RFOD generation by NWZ-3. Therefore, even in the case of normal termination the user should check whether or not more than specified length was used. (This information is always printed out, when RFOD was prepared.)

3. Overflowing the linearization

If between two points of a non-linearly interpolable cross-section set more points than a given limit - NUJM - are required in order to get a linearly interpolable set (with given accuracy), then an error message

n GREATER THAN m IN THE RANGE a,b

is generated and the calculation terminates.

4. Error messages inherited from FEDGROUP-2 [1]

In FEDGROUP-2 there are error messages of the following type:

ERROR IN name NUMBER n

where

name - name of the segment where the error took place
n - error type number

The following, non-fatal, errors are retained in FEDGROUP-3:
302 - argument of the cross-section is not monotonically ascending
351 - required data type is absent
353 - the first energy point is lower than the first data point; cross-section at this point is taken to zero
354 - the last energy point is higher than the highest data point: cross-section is horizontally extrapolated.

5. Convergence messages

If Romberg's integration procedure in CRINT does not converge then the message

POOR CONVERGENCE a,b

is generated where a and b are the upper and lower boundaries of the integration interval, respectively. Normally, this message occurs very rarely and may refer to a singularity in cross-section or flux interpolation.

If Romberg's procedure does not converge in resolved resonance integration an error message

POOR CONVERGENCE IN a,b

is generated, where a and b are the upper and lower boundary of energy interval of integration, respectively. The deviations in integrated values can be printed out if NK=16 is added to the output control number NCOUT.

6. Error messages from the free format input routines

The free-format input routines may give error messages in French. Error may be caused by insufficient input data or by incorrect characters.

7. Further messages

There are other messages which are self explanatory and therefore are not given here.

3.16 ESTIMATION OF DYNAMIC AND OTHER LENGTHS

The discussion of length estimation is followed by the programs:
EVDAUT - no dynamic length is required
PRAFO - length of ToC is

$$LCAT=1+2*NMAT+2*\sum_{i=1}^{NMAT} NTYP_i$$

where NMAT is the number of materials in RFOD, $NTYP_i$ is the number of types of material i on the evaluated file.

An estimation of the length of data headings is the following:
LDH=7*(number of all processed data sets)+6*(number of discrete inelastic excitation levels+number of elastic angular distributions)

In the case of ENDF/B, if all unresolved resonance parameters are energy dependent, the LDH should be enlarged with 7*(number of unresolved resonance series). The dynamic length is estimated by the formula

LFR=2*LC+LCAT+LDH+LDICT+LDAT

where LC is the buffer length, LDICT=3*(number of dictionary's entries), LDAT is the length of nuclear data retained in core during the processing. LDAT is estimated as follows.

If a point-wise cross-section set is processed with NTF=1 then LDAT= =number of data points; if NTF=6 and no linearization is to be performed, then LDAT=0. The linearization brings some uncertainties in length estimation. In the case of UKNDL, LDAT $\leq$ 2*NUJM but for the case of ENDF/B LDAT $\leq$ 2*NDAT *NUJM which may be very large but it is evident that this a very high over-estimation. (NUJM - limit for points between two neighbouring points of a non--linear set,
NDAT - number of points in the non-linearly interpolable set).

In the case of processing resolved resonance parameters:
KEDAK file: LDAT=0
ENDF/B file: LDAT=10*(number of resonances)
In the case of processing unresolved resonance parameters:
KEDAK file: LDAT=0
ENDF/B file: for energy independent case: LDAT=0, for energy dependent case: LDAT=number of energy points.

In the case of processing the angular distribution of elastic scattering the transformation matrix specified on ENDF/B file is placed in the dynamic field thus LDAT=(NMO+1)**2+2*NMO, where NMO is the number of Legendre momenta used for the representation of angular distribution.

In the case of point-wise representation of angular distribution LDAT=0.

NWZ-3

LFR=LSF*LC+NG+1+2*NP+LCAT+LD+LRF1+LRF2+LBLn

where LC is the buffer length

LSF=2 or 1 whether unformatted SFGK or point-wise RFOD to be produced or not
NP=number of spectrum points, if the spectrum is given by formula, then NP=1,
LCAT=length of ToC for the material to be calculated
LD = length of data headings of data types to be used for calculation
LRF1,LRF2 - length of ToC and DH's part of point-wise RFOD to be produced
LBLn - dynamic length required by block n (see 3.6)

RFODS

LFR=LSF*LC+2*LCT+LCD+LRF1+LRF2+LFUN

where

LC is the buffer length
LSF=2 exeept for XMOD='PRNT' when LSF=1
LCT,LCD - length of ToC and DH's part of the input RFOD, respectively
LRF1=comment's length+5+length of ToC for output RFOD
LRF2=length of DH's part for the output RFOD
LFUN=0 except for XMOD='PRNT' where it depends on the NTF of the data to be printed
NTF=1,11 LFUN=MINO(2*NDAT,L)
NTF=6,20 LFUN=NA
NDAT is the number of data points
L is the dynamic length available
NA is the length of a sub-set

SFGKS

LFR=LFS*LC+LMAX+LSET

where

LC is the buffer lenght
LFS=2 except when no new SFGK is produced, (then LFS=1)
LMAX is the maximal length of an input SFGK set (specified by input)
LSET is the maximal length of a produced SFGK set.

3.17 THE MAIN PROGRAM FOR FEDGROUP AND SUMMARY OF FILES TO BE USED IN A FEDGROUP RUN

The main program for the FORTRAN moduls of the FEDGROUP system is

```
COMMON/TOMB/W(<L>)
CALL FEDG3(W,<L>)
END
```

where

W(..) is the dynamic field
<L> is an integer constant,.the length of the dynamic field
FEDG3 is the main control module of the FEDGROUP system calling the control modules of programs

Files used by the FORTRAN modules of the FEDGROUP system

log.n	used by	default	content	remark
5	all		system input	
6	all		system output	
15	FEDG3		card input	
NOUT	all	6	printed output	
NF	PRAFO	1	evaluated data file	
NAUX	PRAFO,NWZ-3	8 or 9	auxiliary file	
NLIB	PRAFO,NWZ-3 RFODS	2	RFOD	
NGL	NWZ-3, RFODS	0	SFGK or auxiliary file	optional
NGK1	SFGKS	3	SFGK to be manipulated	
NGK2	SFGKS	2	SFGK produced	optional
NPOINT	NWZ-3	8	point-wise RFOD	

4. TEST CALCULATIONS WITH FEDGROUP-3

4.1 FORMAL TESTING

The work of the programs EVDAUT, PRAFO, RFODS, SFGKS can be checked easily by printing out the resulting evaluated data, RFOD and SFGK files, respectively and comparing them with the outgoing files. A more complicated method of formal testing - cross-testing - can be applied to the NWZ-3 program. That is certain types of group constants can be calculated in different ways and the results should be exactly or approximately the same. Here some proposed cross-testings are given.

1. A point-wise cross-section set can be processed as an RFOD's set having either NTF=1 or NTF=6. The results must be exactly the same.

2. The average cosine of elastic scattering can be calculated either by integrating and averaging the angular distribution of elastic scattering (block 2) or by calculating the elastic group transfer matrix elements up to P_1 (block 6 and 7) and taking

$$\mu_i = \frac{\sum_{j=i}^{j+k} \sigma_1^{i\to j}}{\sum_{j=i}^{j+k} \sigma_o^{i\to j}}$$

If the elastic scattering does not depend on energy in the group interval then the two μ's should be approximately the same.

Some files contain the average scattering cosine as a function of energy. This can also be group-averaged (block 1) and compared with those calculated in on other way. In the case of ENDF/B data an approximate agreement can be expected. In the case of KEDAK data, due to the different evaluation [5], agreement cannot be expected in each case.

3. If the total inelastic cross-section and level inelastic cross-section are given on a file then the group-averaged total inelastic cross-section can be calculated either by block 1 or block 3. The two results should be exactly the same if the total inelastic cross-section is exactly equal to the sum of level cross-sections at every energy point.

4. The infinite diluted cross-sections calculated by block 4 are exactly the same as those calculated by block 1.

5. The sum of the P_o elastic transfer matrix elements is approximately equal to the group averaged elastic scattering cross-section. The less lethargy mesh the better the approximation. If the scattering cross-section is energy independent this equality is exact.

6. The work of blocks 8 and 9 can be checked by processing the point-wise cross-sections to group-averaged cross-sections. For block 8 this is performed either by block 1, or 6, in the case of block 9 only by block 6.

7. As is known from 3.3 there may be two different representations of energy dependent unresolved parameters. The first (NTF=20) is typical for

KEDAK data, the second is typical for ENDF/B data. By means of an ad-hoc interface program a data set of the first type could be transformed to the representation of the second type and by this the same group constants can be calculated in two different ways. Unfortunately, no formal testing can be recommended for resolved resonance calculation.

The above described method of formal testing was of great help in eliminating the programming errors.

4.2 COMPARISON OF THE CALCULATED GROUP CONSTANTS WITH THOSE PRODUCED BY OTHER CODES FROM THE SAME DATA SET

All test calculations were performed for the 26-group ABBN system, the energy boundaries of which are: 10.5 MeV, 6.5 MeV, 4.0 MeV, 2.5 MeV, 1.4 MeV, 800 keV, 400 keV, 200 keV, 100 keV, 46.5 keV, 21.5 keV, 10.0 keV, 4.65 keV, 2.15 keV, 1.0 keV, 465.0 eV, 2.15 eV, 100.0 eV, 46.5 eV, 21.5 eV, 10.0 eV, 4.65 eV, 2.15 eV, 1.0 eV, 0.465 eV, 0.215 eV, 10^{-3} eV. [11].

1. Comparison with the sample calculation given in the MIGROS-3 report [5]. (KEDAK data).

These sample calculations relate the elements U-235 and O-16.

In the Table 4.1 group averaged infinite diluted cross-sections and f-factors are presented for unresolved (14th group) and for resolved (18 th) cases. Constants in the resolved energy range are calculated with 1 % accuracy. However in some cases the deviation is somewhat larger. The agreement is better if more resonances are taken (NRES=30). In MIGROS-3 no correction for resonance width is taken into account, i.e. MIGROS-3 calculates as if γ_r=1 every where. The values in the column FEDGROUP-3 (M) arose from a modification of the program by taking γ_r=1 for each resonance.

In the unresolved region the group-averaged cross-sections depends on the number of mesh points taken in the group interval. In MIGROS-3 the end points and the middle of the group lethargy interval is taken. This corresponds to NLETH=2.

In Table 4.2 the inelastic scattering transfer probabilities calculated with MIGROS-3 and FEDGROUP-3 are compared.

The formula for discrete level inelastic scattering used in [5] is somewhat different from that of FEDGROUP-3. MIGROS-3 uses the formula (6.3) of ref [5] where as FEDGROUP-3 uses formula (6.4). For the sake of comparison FEDGROUP-3 was modified to use formula (6.3), too. Therefore two FEDGROUP results are given for the group 5. There is appreciable deviation of results only for the lower inscattering group. This is due to the lower precision used in FEDGROUP-3. Moreover, in FEDGROUP-3 a cut-off is applied for lower inscattering groups because there is no sense in taking into account these transmissions for the inaccuracy of level energies which give rise to an enormous uncertainties for this transfer elements.

In Table 4.3 the elastic scattering matrix of O-16 up to momentum P_3 is compared for the 3rd and 12th ABBN groups. As the transfer matrix elements and not the probabilities are compared, the values given in [5] are multiplied by the elastic scattering group cross-sections, i.e. by 2.04014 and 3.70, respectively. It seems that FEDGROUP-3 agrees with MIGROS-3 only in the 12th group. The poor agreement in group 3 may be due to the following reasons:

- MIGROS-3 applies a correction procedure for the angular distribution in order to get back the average cosine given in the KEDAK file. This is not done in FEDGROUP-3.

- FEDGROUP-3 takes into account the variation of the elastic scattering cross-section within the group energy interval.

2. Calculation with UKNDL data

For comparison the results of calculation given in [12] are used. The data set underlying the comparison was that for U-238 (DFN=401). The 26-group infinite diluted cross-sections are compared with each other in Table 4.4. It is seen that the group averaged cross-sections are in good agreement except the resonance groups (groups 13-22) where 1-2% deviation can be observed. The reason for these deviations is not clear. (It may be due to the different accuracy of the interpolation and integration methods).

The group averaged μ, however are quite different. A direct investigation of the angular distribution of elastic scattering of U-238 shows that there is an increased back-scattering in the energy region corresponding to groups 6 and 7 and this inevitably leads to an average cosine less than that for isotropic scattering.

In Table 4.5 the calculated f-factors are compared. At least within the accuracy given in [12], the agreement is perfect.

3. Calculation with ENDF/B data

The evaluated data set for U-235 from the ENDF/B-IV file (MAT=1261) is used for testing the calculation of infinite diluted group averaged cross--sections for the resolved and unresolved resonance regions. The infinite diluted group averaged constants for total, elastic, (n,γ) and fission cross--sections have been calculated for the 10-24 groups of the ABBN system. For comparison, the same quantities from [13] are taken, where the calculation was performed by the RESEND code [14]. The fission constants are also compared with those calculated by the FOUR-ACES code [15] (Table 4.6).

It should be noted that for this data set the constants in the unresolved region strongly depending on the lethargy mesh. In Table 4.7 the total elastic, (n,γ) and fission constants are presented as a function of the number of lethargy interval - NLETH - in the group interval. It can be seen the values are stabilized only about NLETH=20. Therefore in our calculation 20 lethargy intervals per group were used.

When comparing the results with those of FOUR-ACES, it should be noted that this code adds the back-ground cross-sections to the resonance ones after their averaging., where as FEDGROUP-3 does this before averaging.

According to the formal testing discussed in 4.1.2 a calculation is made for the group averaged cosine of C-12 (MAT=1274). For comparison the results of Garg [13] are also used. In Table 4.8 are given (1) - Garg's results, (2) - group-averaged μ, (3) - integrated angular distribution (block 2), (4) - from elastic transfer matrix elements (block 7 and 6).

TABLE 4.1 U-235 KEDAK DATA, T=300K

	14TH GROUP		18TH GROUP		
	MIGROS-3	FEDGROUP-3	MIGROS-3	FEDGROUP-3	FEDGROUP-3(M) FEDGROUP-3(NRES=30)
	1.2281E1	1.2255E1	1.2886SE1	1.27181E1	1.27181E1 1.28317E1
	2.9597	2.9795	2.31701E1	2.30609E1	2.30609E1 2.31259E1
	6.6534	6.6880	2.89997E1	2.88744E1	2.88744E1 2.89599E1
(0)	0.9850	0.9849	0.94397	0.9413	0.9409 0.9422
(0)	0.8061	0.8019	0.42534	0.3952	0.4201 0.4243
(0)	0.8117	0.8084	0.44213	0.4117	0.4363 0.4408
(100)	0.9966	0.9965	0.97010	0.9703	0.9697 0.9699
(100)	0.9611	0.9591	0.71647	0.7143	0.7158 0.7169
(100)	0.9630	0.9614	0.72498	0.7230	0.7240 0.7251
(1.E4)	0.9999	1.0000	0.9991	0.9998	0.9998 0.9998
(1.E4)	0.9995	0.9995	0.99289	0.9940	0.9938 0.9939
(1.E4)	0.9995	0.9995	0.9932	0.9937	0.9936 0.9936

TABLE 4.2 INELASTIC SCATTERING MATRIX; KEDAK DATA

GROUP TO	4 MIGROS-3	4 FEDGROUP-3	5 MIGROS-3	5 FEDGROUP-3	5 FEDGROUP-3(M)
1	1.273E-5	1.278E-5			
2	1.658E-3	1.641E-3			
3	2.587E-2	2.579E-2			
4	1.609E-1	1.606E-1			
5	2.859E-1	2.858E-1	2.764E-1	2.637E-1	2.762E-1
6	3.045E-1	3.047E-1	5.249E-1	5.345E-1	5.249E-1
7	1.481E-1	1.483E-1	1.677E-1	1.701E-1	1.678E-1
8	5.197E-2	5.207E-2	2.321E-2	2.368E-2	2.327E-2
9	1.616E-2	1.620E-2	5.944E-3	6.067E-3	5.970E-3
10	3.838E-3	3.848E-3	1.427E-3	1.453E-3	1.431E-3
11	8.532E-4	8.556E-4	3.504E-4	3.559E-4	3.509E-4
12	1.882E-4	1.892E-4	9.537E-5	9.661E-5	9.543E-5
13	4.120E-5	4.130E-5	2.963E-5	2.944E-5	2.964E-5
14	8.817E-6	8.836E-6	1.042E-5	1.050E-5	1.042E-5
15	1.911E-6	1.914E-6	4.154E-6	4.180E-6	4.155E-6
16	4.150E-7	4.151E-7	1.790E-6	1.800E-6	1.791E-6
17	8.847E-7	8.792E-7	7.911E-7	7.952E-7	7.914E-7
18	1.914E-8	1.907E-8	3.611E-7	3.623E-7	3.612E-7
19	4.153E-9	4.102E-9	1.672E-7	6.758E-8	1.673E-7
20	8.849E-10	8.401E-10	7.660E-8	0.	2.170E-8
21	1.915E-10	1.840E-10	3.557E-8	0.	0.
22	4.153E-11	3.583E-11	1.660E-8	0.	0.
23	8.849E-12	5.480E-12	7.635E-9	0.	0.
24	1.915E-12	0.	3.551E-9	0.	0.
25	4.153E-13	0.	1.659E-9	0.	0.
26	1.129E-13	0.	1.420E-9	0.	0.

TABLE 4,3 P0,P1,P2,P3 ELASTIC SCATTERING MATRIX (KEDAK DATA)

	3 → 3		3 → 4		12 → 12		12 → 13	
L	MIGR-3	FEDG-3	MIGR-3	FEDG-3	MIGR-3	FEDG-3	MIGR-3	FEDG-3
0	1,803	1,815	0,2376	0,2245	3,1153	3,1153	0,5842	0,5847
1	0,6064	0,4812	-0,0570	-0,0507	3,3256	3,3319	-0,1783	-0,1776
2	0,3901	0,3955	1,95E-3	6,25E-4	1,262E-2	1,264E-2	-9,66E-3	-9,72E-3
3	0,1771	0,1730	1,065E-3	9,95E-3	1,48E-4	3,08E-4	-1,48E-4	3,32E-4

TABLE 4,4 GROUP AVERAGED CROSS-SECTION FOR U-238 (UKNDL DATA, DFN=401)

	σ_t		σ_e		σ_γ		μ	
	[12]	FEDGROUP-3	[12]	FEDGROUP-3	[12]	FEDGROUP-3	[12]	FEDGROUP
1	6,468	6,468	3,491	3,491	6,847E-3	6,847E-3	8,473E-1	3,879E-2
2	7,712	7,712	4,569	4,569	1,181E-2	1,181E-2	8,143E-1	5,203E-2
3	7,899	7,899	4,649	4,649	2,442E-2	2,442E-2	7,309E-1	2,565E-2
4	7,333	7,333	3,863	3,863	6,355E-2	6,355E-2	5,577E-1	1,673E-2
5	6,980	6,980	4,433	4,433	1,466E-1	1,466E-1	4,259E-1	1,439E-2
6	8,234	8,234	6,364	6,364	1,368E-1	1,368E-1	3,450E-1	-4,953E-3
7	9,944	9,944	8,506	8,506	1,362E-1	1,362E-1	2,499E-1	-2,917E-3
8	11,51	11,51	10,51	10,51	1,706E-1	1,706E-1	1,529E-1	-2,917E-2
9	12,69	12,69	12,29	12,29	2,838E-1	2,836E-1	8,467E-2	-2,444E-2
10	13,79	13,79	13,31	13,31	4,807E-1	4,807E-1	3,436E-2	-8,206E-3
11	14,47	14,47	13,81	13,81	6,642E-1	6,645E-1	9,902E-3	3,517E-4
12	15,25	15,25	14,40	14,40	8,567E-1	8,565E-1	2,801E-3	2,825E-3
13	16,47	16,62	15,47	15,60	9,838E-1	1,003	2,801E-3	2,825E-3
14	19,21	19,06	17,65	17,52	1,540	1,523	2,801E-3	2,825E-3
15	20,84	20,86	17,92	17,94	2,896	2,902	2,801E-3	2,825E-3
16	20,15	20,12	16,17	16,16	3,933	3,914	2,801E-3	2,825E-3
17	84,55	84,73	64,24	64,36	20,27	20,33	2,801E-3	2,825E-3
18	37,82	37,88	22,60	22,63	15,14	15,18	2,801E-3	2,825E-3
19	127,3	126,8	71,49	71,25	55,65	55,45	2,801E-3	2,852E-3
20	109,3	109,4	32,15	32,14	77,08	77,20	2,801E-3	2,852E-3
21	186,7	187,1	18,39	18,42	168,1	168,5	2,801E-3	2,852E-3
22	9,038	9,039	8,347	8,346	6,852E-1	6,862E-1	2,801E-3	2,825E-3
23	9,368	9,368	8,871	8,872	4,960E-1	4,960E-1	2,801E-3	2,825E-3
24	9,587	9,587	8,988	8,989	5,987E-1	5,985E-1	2,801E-3	2,825E-3
25	9,655	9,655	8,837	8,836	8,181E-1	8,182E-1	2,801E-3	2,852E-3
26	10,74	10,64	8,010	5,873	2,73	4,76	2,801E-3	2,825E-3

TABLE 4,5 f-FACTORS FOR U-238 (UKNDL DATA DFN=401)
T=300K, SIGMA0=100,

	f_t		f_e		f_γ	
	[12]	FEDGROUP-3	[12]	FEDGROUP-3	[12]	FEDGROUP-3
15	0,58	0,58	0,71	0,71	0,48	0,47
16	0,64	0,64	0,79	0,79	0,37	0,37
17	0,16	0,16	0,25	0,25	0,13	0,13
18	0,28	0,28	0,46	0,46	0,14	0,14
19	0,11	0,11	0,19	0,19	0,08	0,08
20	0,09	0,09	0,26	0,26	0,06	0,06
21	0,08	0,085	0,51	0,51	0,08	0,084

TABLE 4,6 GROUP AVERAGED CROSS-SECTION FOR U-235 (ENDF/B DATA)

GROUP	σ_t		σ_e		σ_γ		σ_f		
	GARG	FEDGROUP-3	GARG	FEDGROUP-3	GARG	FEDGROUP-3	GARG	PANINI	FEDGROUP-3
4	7,001	7,093	3,965	4,076	0,054	0,059	1,291	1,267	1,267
5	6,727	6,85	4,001	4,106	0,0984	0,109	1,216	1,220	1,220
6	7,476	7,942	5,015	5,462	0,145	0,163	1,162	1,162	1,162
7	9,267	9,482	6,975	7,172	0,225	0,250	1,286	1,279	1,279
8	11,08	10,99	8,685	8,661	0,3931	0,368	1,513	1,475	1,475
9	12,383	12,52	9,780	10,10	0,6075	0,531	1,854	1,749	1,749
10	13,66	13,84	10,60	11,00	0,8046	0,754	2,237	2,048	2,06
11	14,62	15,21	10,78	11,48	1,023	1,086	2,24	2,59	2,64
12	16,02	16,76	11,01	11,79	1,318	1,444	3,695	3,426	3,53
13	18,24	18,72	11,199	11,88	1,867	1,78	5,178	5,047	5,061
14	22,07	22,65	11,464	12,19	3,208	3,06	7,394	7,154	7,40
15	27,19	28,67	11,535	12,38	4,642	4,676	11,01	11,68	11,60
16	33,91	35,90	11,531	12,53	6,610	7,119	15,77	16,59	16,25
17	44,15	45,78	11,519	12,60	10,555	12,07	22,08	21,24	21,11
18	62,78	63,13	12,312	11,88	15,44	16,32	35,03	34,72	34,96
19	79,44	78,86	12,315	12,52	23,998	23,73	43,122	42,34	42,64
20	108,31	107,89	12,273	12,79	44,838	44,54	51,199	49,91	50,54
21	96,99	96,09	11,05	11,74	37,43	36,98	48,51	46,31	47,34
22	35,88	36,17	11,41	12,67	7,13	6,84	17,34	14,80	16,64
23	60,87	61,38	12,545	13,83	12,398	12,19	35,93	34,78	35,34
24	86,294	86,60	13,648	13,41	7,17	7,13	65,48	66,12	66,10
25	205,92	206,86	14,672	14,41	34,30	34,10	156,95	158,5	158,4

TABLE 4,7 INFINITE DILUTED CROSS-SECTION IN UNRESOLVED RANGE AS A FUNCTION OF LETHARGY MESH (U-235 FROM ENDF/B FOR 14TH GROUP OF ABBN SYSTEM)

NLETH	σ_t	σ_e	σ_γ	σ_f
2	22,248	12,20	3,311	6,734
4	22,09	12,14	3,059	6,894
5	22,85	12,18	3,032	7,634
6	22,47	12,16	3,026	7,279
7	22,54	12,17	3,035	7,336
8	22,59	12,18	3,046	7,363
9	22,69	12,19	3,069	7,433
10	22,70	12,19	3,045	7,470
11	22,61	12,21	3,129	7,275
12	22,49	12,17	3,036	7,287
13	22,81	12,23	3,144	7,437
14	22,67	12,18	3,030	7,464
15	22,74	12,23	3,156	7,356
16	22,55	12,17	3,029	7,350
17	22,65	12,21	3,120	7,324
18	22,60	12,18	3,045	7,376
19	22,64	12,20	3,092	7,347
20	22,65	12,19	3,060	7,40
21	22,62	12,19	3,074	7,359
22	22,64	12,19	3,079	7,377
23	22,59	12,18	3,056	7,349
24	22,63	12,19	3,080	7,353
25	22,56	12,18	3,048	7,330

TABLE 4,8 AVERAGE COSINE FOR C-12, CALCULATED IN THREE DIFFERENT WAY

GROUP	[13]	1	2	3
1	0,388	0,4237	0,4237	0,42,88
2	0,215	0,2927	0,2925	0,2932
3	0,022	0,0292	0,0290	0,315
4	0,093	0,0878	0,0875	0,0889
5	0,126	0,1252	0,1248	0,1247
6	0,111	0,1101	0,1097	0,1092
7	0,090	0,0888	0,0885	0,0883
8	0,075	0,0729	0,0725	0,0724
9	0,066	0,0645	0,0642	0,0642
10	0,061	0,0603	0,05997	0,05996
11	0,058	0,05832	0,05801	0,05798
12	0,058	0,05733	0,05702	0,05604

5. SOME INPUT EXAMPLES

Input cards for FEDGROUP-3 runs are presented and discussed here. Note that the namelist input cards are (with one exception) at the same time, control cards for the system's run. The entrance in a control module activates the default values of parameters. Changes in the parameters, relative to their default values are specified on the namelist input cards which are discussed here.

Example 1 In this example, we present preparation of RFOD from an ENDF/B data set, calculation of finite diluted group averaged cross-section, Greuling-Goertzel constants, inelastic scattering matrix, resonance shielded-group averaged constants and elastic group transfer matrix for some groups. The input cards are given in Table 5.1 and are discussed below:

Cards 1 NPRAF=3 calls for the PRAFO of the ENDF/B file; the ToC length and DHs length enlarged relative to the default ones; only the input namelist cards will be printed out and log. number 9 used for the auxiliary file.

2 comment part of the RFOD

3 material name on the evaluated data file MAT=1274; on RFOD the name MATN=60012 is assigned; two dictionary table entries will be modified

4 the modification entries (in free-format)

5 no more material will be processed (control effect of MATF=-1)

6 Processing with NWZ-3 begins; log. number 3 used for SFGK; input namelist cards, group boundaries and RFOD ToC will be printed;

7 spectrum defined by formula is used; if the default spectrum function is used then the joining point of fission and 1/E spectra is 10^8 eV, that is, 1/E spectrum averaging is used.

8 ABBN group system is used

9-10 temperatures and σ_o-s are specified

11 MATN=60012 is calculated (conventionally, this is C-12)

12 group constants for elastic scattering cross-section are calculated for the whole group system

13 Greuling-Goertzel constants are calculated for groups 5-10

14 inelastic scattering matrix is calculated for the whole group system

15 infinite diluted and self-shielded cross-section are calculated (total, (n,γ), elastic and fission) for groups 3-7

16 return to the main control module (control effect of NTNAM=0)

17 log. number 9 is used as auxiliary file for point-wise RFOD calculation

18 ABBN group system is used

19 MATN=60012 is calculated

20 elastic scattering cross-sections covering the energy range 90 keV-1.1 MeV are taken from the original RFOD and written to a new point-wise RFOD

21 elastic transfer probabilities to groups 6-8 for zero and first momenta are calculated

22 the point-wise RFOD is finished (control effect of NTNAM=-1)

23 input RFOD will be on log. number 8 (this is the RFOD prepared previously)

24 ABBN group constant system is used

25 spectrum defined by formula is used

26 MATN=60012 is calculated

27 elastic scattering matrix for groups 6-7 is calculated

Example 2 In this example an earlier prepared RFOD for U-235 is used. Point-wise cross-sections are calculated in two energy intervals in the resonance region. The two data sets are merged in one RFOD data set. The input cards are given in Table 5.2 and are discussed below:

1 log. number 3 is used as auxiliary file; the input cards and the generated RFOD is to be printed out

2-3 Temperature value is specified

4 MATN=920235 i.e. U-235 is calculated

5-6 point-wise cross-sections in the ranges 3-4 eV and 4-6 eV, respectively are to be calculated; the relating NTNAM's, because of the further processing, are descending. Note: the log. number of point-wise RFOD will be 8 (default)

7 the pont-wise RFOD is finished (control effect of NTNAM=-1)

8 a new RFOD will be constructed from RFOD on log. number 8; auxiliary file: log. number 3.

9 comments for the new RFOD

10 the point-wise data sets on input RFOD are merged, (new RFOD arises in the place of the old one)

11 the new RFOD on log. number 8 is printed out

Example 3 In this example resonance parameters of a material (U-235) are selected from an RFOD and printed out. The input cards are given in Table 5.3 and are discussed below:

1 a new RFOD will be constructed, log. number of the auxiliary file is 3

2 comment for the new RFOD

3 material(s) and data type(s) to be specified below will be copied

4 material and data types to be copied (in free-format)

5 the new RFOD is finished and written into the file log. number 8

6 RFOD on log. number is printed out

Example 4 In this example setting out from a previously prepared RFOD on SFGK file with some data sets is constructed, thereafter the SFGK sets are merged

The input cards are given in Table 5.4 and are discussed below:

1 SFGK set will be on log. number 3; input cards and group boundaries will be printed out; the task identifier will be 1; the buffer length will be 878 (because this may be matched better to the disk track capacity)

2 averaging spectrum is defined by formula; in default case the joining point of fission and 1/E spectra is at 10^8 eV

3 group boundaries will be specified by input

4 number of groups and group boundaries (in free-format)

5-6 temperature and σ_o parameters

7 MATN=80016 that is O-16 will be calculated

8-9 group-averaged self-shielded infinite diluted cross-section calculated for groups 1-3 and 4-6, respectively; as normal point-wise (no background) cross-sections and resonance parameters are given on the file, the region boundaries should be changed to 0.

10-12 the total group averaged cross-sections are calculated for the groups 2-4, 1, 5-6, respectively

13 return to main control module (control effect of NTNAM=0)

14-15 are equivalent with 5-6

16 a table of contents from the SFGK file is printed; buffer length: 878

17 SFGK sets having ID=80016, 5152, 4, 1 are to be merged and written to the file log. number 9; number of groups 6; buffer length: 878 the input cards and the merged SFGK sets are printed

18 the same merging is performed with SFGK sets ID=80016, 1001, 1, 1,

19 manipulation with SFGK file is terminated

TABLE 5.1 INPUT CARDS FOR EXAMPLE 1

```
&PRAF NPRAP=3,LCAT=200,LDH=2500,NCOUT=1,NAUX=9&END                    -------1
 C-12  ENDF/B-IV  MAT=1274                                            -------2
&MAT MATF=1274,MATN=60012,NDICT=2&END                                 -------3
 3003  1003  0  3101  1101  0                                         -------4
&MAT MATF=-1&END                                                      -------5
&CTRL NCOUT=11,NGL=3&END                                              -------6
&SPEC X='FORMULA ',PK=1,E8&END                                        -------7
&GROU X='BANB    '&END                                                -------8
&TSGO NT=1,NSI=2&END                                                  -------9
 0.  0.  10.                                                          -------10
&MATE MATN=60012&END                                                  -------11
&TYPE NTNAM=1002,NFEL=1&END                                           -------12
&TYPE NTNAM=2002,NFEL=2,NR=5,10&END                                   -------13
&TYPE NTNAM=1005,NFEL=3,NR=1,26&END                                   -------14
&TYPE NTNAM=5152,NFEL=4,NR=3,7&END                                    -------15
&TYPE NTNAM=0&END                                                     -------16
&CTRL NGL=9&END                                                       -------17
&GROU X='BANB    '&END                                                -------18
&MATE MATN=60012&END                                                  -------19
&TYPE NTNAM=1002,NFEL=8,NG=0,ER=9,E4,1,1E6,NT=1&END                   -------20
&TYPE NTNAM=2002,NFEL=7,NR=6,8,NT=2,NG=26&END                         -------21
&TYPE NTNAM=-1&END                                                    -------22
&CTRL NLIB=8&END                                                      -------23
&GROU X='BANB    '&END                                                -------24
&SPEC X='FORMULA ',PK=1,E8&END                                        -------25
&MATE MATN=60012&END                                                  -------26
&TYPE NTNAM=2002,NFEL=6,NR=6,7&END                                    -------27
```

TABLE 5.2 INPUT CARDS FOR EXAMPLE 2

```
&CTRL NGL=3,NCOUT=5&END                                                  -------1
&TSGO NT=1&END                                                           -------2
 0,                                                                      -------3
&MATE MATN=920235&END                                                    -------4
&TYPE NFEL=9,ER=3,,4,,NTNAM=5153&END                                     -------5
&TYPE ER=4,,6,,,NTNAM=5153&END                                           -------6
&TYPE NTNAM=-1&END                                                       -------7
&RFOD XMOD='BEGN',NLIB=8,NGL=3&END                                       -------8
  UNIFIED POINT-WISE RFOD                                                -------9
&RFOD XMOD='UNIF'&END                                                    ------10
&RFOD NLIB=8,NCOUT=5,XMOD='PRNT'&END                                     ------11
```

TABLE 5.3 INPUT CARDS FOR EXAMPLE 3

```
&RFOD XMOD='BEGN',NGL=9&END                                              -------1
 U-235 RESONANCE PARAMETERS                                              -------2
&RFOD XMOD='INCL'&END                                                    -------3
 920235  2  5152  5155                                                   -------4
&RFOD XMOD='FINS',NLIB=8&END                                             -------5
&RFOD XMOD='PRNT',NLIB=8,NCOUT=4&END                                     -------6
```

TABLE 5.4 INPUT CARDS FOR EXAMPLE 4

```
&CTRL NGL=3,NCOUT=3,KDAT=1,LC=878&END                                    -------1
&SPEC X='FORMULA ',PK=1,E8&END                                           -------2
&GROU &END                                                               -------3
 6   5.E6   1.E6   5.E5   1.E5   5.E4  1.E3   1.E2                        -------4
&TSGO NT=1,NSI=2&END                                                     -------5
 0,  0, 100,                                                             -------6
&MATE MATN=80016&END                                                     -------7
&TYPE NFEL=4,NTNAM=5152,NR=1,3,EL=0.,,0.,,EU=0.,,0,&END                  -------8
&TYPE NR=4,6&END                                                         -------9
&TYPE NR=1,6,NFEL=3,NTNAM=1005&END                                       ------10
&TYPE NTNAM=1001,NFEL=1,NR=2,4&END                                       ------11
&TYPE NR=1,1&END                                                         ------12
&TYPE NR=5,6&END                                                         ------13
&TYPE NTNAM=0&END                                                        ------14
&TSGO NT=1,NSI=2&END                                                     ------15
 0,  0, 100,                                                             ------16
&SFGK FUNC='EXPLORE ',LC=878&END                                         ------17
&SFGK FUNC='COMPLETE',LC=878,NGK2=9,NG=6,NCOUT=9,ID=80016,5152,          ------18
  4,1&END
&SFGK ID=80016,1001,1,1,0,0&END                                          ------19
&SFGK FUNC='FINISH  '&END                                                ------20
```

REFERENCES

[1] P. Vértes, A Program System for Producing Group Constants from Evaluated Nuclear Data of Files Disseminated by IAEA INDC(HUN)-13/L+Sp (1976)

[2] D. Woll, Card-Image Format of the Evaluated Nuclear Data File KEDAK, KFK-880, 1968

[3] K. Parker, The Aldermaston Nuclear Data Library as at May 1963, AWRE O-70/63, 1963

[4] ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF (Revised by D. Garber, C. Dunford and S. Pearlstein) October 1975

[5] I. Broeders, B. Krieg, MIGROS-3; A Code for the Generation of Group Constants for Reactor Calculations from Neutron Nuclear Data in KEDAK Format KFK 2388, 1977

[6] M.F. James, Recommended Formulae and Formats for a Resonance Parameter Library AEEW - R 621, Dorset, 1968

[7] Z. Szatmary, J. Valko, GRACE - Multigroup Fast Neutron Spectrum Code KFKI-70-14 RPT (1970)

[8] P. Vértes, Nuclear Science and Engineering 52, 485 (1973)

[9] G. Szwarzbaum, M. Segev, S. Yiftah; Inelastic Scattering Matrices for Fast Neutron Calculation IA-899, 1964

[10] Program MERCURE-IV, CPL program documentation

[11] I.I. Bondarenko, M.N. Nikolayev, L.P. Abagyan and N.O. Bazazyantz, Group Constants for Reactor Calculation Moscow, Atomizdat, 1964

[12] E. Menapace, M. Motta, G.C. Panini, A 26-Group Library with Self--Shielding Factors for Fast Reactor Calculations from the UK Nuclear Data File RT/FI(73)15 Bologna

[13] S.B. Garg, A 27-group Cross-Section Set Derived from ENDF/B Library, INDC(IND)-21/G+Sp

[14] O.Ozer, RESEND: A Program to Preprocess ENDF/B Materials with Resonance Files into a Pointwise Form, BNL 17134 (1973)

[15] G.C. Panini, private communication

[16] R. Goldstein, Nuclear Science and Engineering, 13, 132 (1962)

[17] G. Forti, Nuclear Science and Engineering 19, 449 (1964)

[18] N.M. Greene et al, AMPX: An Interfaced System to Generate Coupled Multigroup Neutron-Gamma Cross-sections from ENDF/B, ORNL-TM-3706

APPENDIX

The FEDGROUP-3 code package /for IBM-OS360/

FEDGROUP-3 can be distributed on magnetic tape containing 17 files, presented in Table A1.

The first file contains assembler routines taken from the code package MERCURE-IV, facilitating the free-format input. It consists of 11 assembler programs and before each a control card for the IEBUPDTE utility is placed in order to facilitate the creation of a partitioned data set of which each assembler program is a member. By means of this partitioned data set, it is easy to compile the assembler routines one-by-one.

The second file contains the FORTRAN auxiliary routines for the free--format input taken also from the code package MERCURE-IV.

The third file contains all the FORTRAN routines of the FEDGROUP-3 system.

The 4th file contains the overlay control cards

The 5th file contains the PL/1 program EVDAUT.

The 6th file contains job control cards required for a FEDGROUP-3 run. It is assumed that the first three files of the package are already compiled and available as an object modele /SYSLIN/. A step with EVDAUT for file preparation may also precede these cards.

Files 7-10 contain the input data for four FEDGROUP sample calculations; files 11-13 are further files required for these calculations.

File 11 contains ENDF/B data for carbon, required for the first sample calculation. File 12 is used in the second and third sample calculations, containing data for U-235 in RFOD form. File 13 is used in the fourth sample run, containing data for O-16 in RFOD form.

Files 14-17 contain the corresponding output for the sample calculations.

The FEDGROUP-3 package

Table A1

File	content	mode	DSNAME	Number of records	RECFM	BLKSIZE	LRECL
1	Assembler free-format input routines	EBCDIC	INP.ROU.ASS	1347	FB	800	80
2	FORTRAN free-format input routines	BCD	INP.ROU.FORT	619	FB	800	80
3	FEDGROUP-3 source	BCD	FG.SOURCE	8730	FB	800	80
4	FEDGROUP-3 overlay control cards	EBCDIC	FGOVL	73	FB	800	80
5	EVDAUT program	EBCDIC	EVDAUT	85	FB	800	80
6	Job cards	EBCDIC	JCL	27	FB	800	80
7	Sample input-1	EBCDIC	SAMPLE.INP1	27	FB	800	80
8	Sample input-2	EBCDIC	SAMPLE.INP2	11	FB	800	80
9	Sample input-3	EBCDIC	SAMPLE.INP3	6	FB	800	80
10	Sample input-4	EBCDIC	SAMPLE.INP4	21	FB	800	80
11	ENDF/B file for C-12	EBCDIC	C12EN	2040	FB	8000	80
12	RFOD for U-235	binary	U235RF	19	VBS	3608	3604
13	RFOD for O-16	binary	O16RF	15	VBS	3520	3516
14	Sample output-1	list	SAMPLE.OUT1	283	U	121	
15	Sample output-2	list	SAMPLE.OUT2	438	U	121	
16	Sample output-3	list	SAMPLE.OUT3	302	U	121	
17	Sample output-4	list	SAMPLE.OUT4	326	U	121	

APPENDIX B. ON THE GOLDSTEIN FACTOR

An other possible definition of the group-averaged Goldstein factor is

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

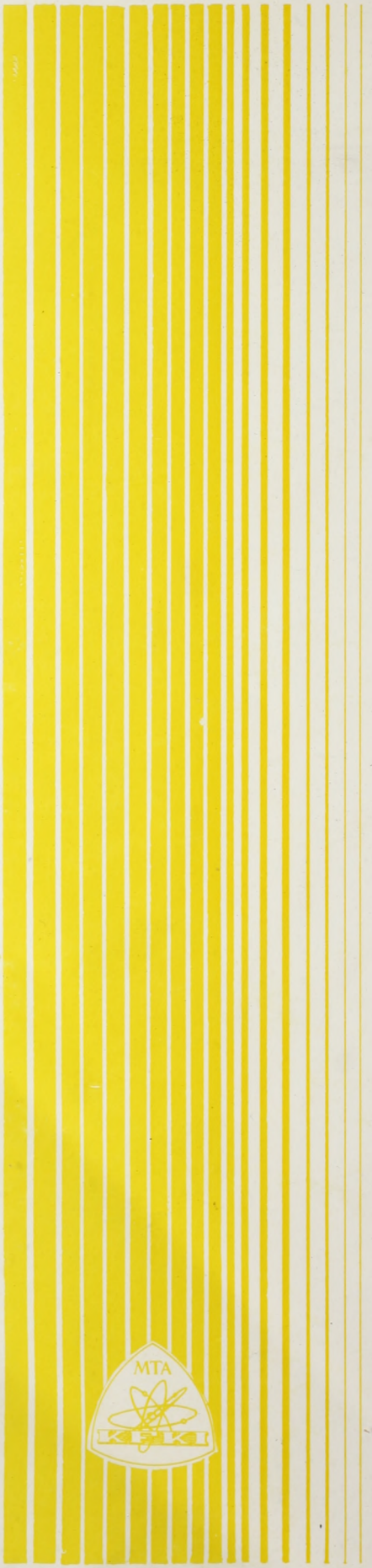
where

$$\gamma(E) = \sum_{r=1}^{NR} \gamma_r\ Z_r(E)$$

$$Z_r(E) = \begin{cases} 1 & \text{if } E_{r-1} < E \leq E_r \\ 0 & \text{otherwise} \end{cases}$$

E_r is the energy of the r-th resonance.

63.147



Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Gyimesi Zoltán
Szakmai lektor: Kereszturi András
Nyelvi lektor: Shenker Harvey
Gépelte: Balczer Györgyné
Példányszám: 410 Törzsszám: 81-301
Készült a KFKI sokszorosító üzemében
Felelős vezető: Nagy Károly
Budapest, 1981. május hó