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KFKI-71-4 INDC(HUN)-002/G P. Vértes PRODGROUP - A PROGRAM FOR THE PRODUCTION OF MULTIGROUP REACTOR CONSTANTS FROM THE EVALUATED NUCLEAR DATA AVAILABLE AT IAEA Hungarian Academy of Sciences CENTRAL RESEARCH INSTITUTE FOR PHYS BUDAPEST

KFK1-71-4

PRODGROUP - A PROGRAM FOR THE PRODUCTION OF MULTIGROUP REACTOR CONSTANTS FROM THE EVALUATED NUCLEAR DATA AVAILABLE AT IAEA

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1. Introduction

The recent development of reactor calculations in our country [1] has required a reliable set of group constants. In the published literature there can be found some sets of microgroup constants, as, e.g. [2], [3], etc. These constants have been produced from evaluated nuclear data which originally resulted from nuclear theory and experiments. The group constants sets have been published over a relatively long period of time and they are not flexible enough as far as the calculation methods and special cicumstances are concerned, e.g. diffusion, transport and Monte Carlo calculation, heterogeneous systems, shielding calculations, etc.

Recently, evaluated data of some isotopes which are important in reactor physics have become available at IAEA on magnetic tape file. Therefore, to avoid the difficulties with the readymade group constants, a program has been prepared for their calculation from these evaluated data. It is hoped that in the future the accuracy of the nuclear data and the assortment of material available at IAEA will grow, thereby satisfying requirements concerned with the group constants in reactor physics calculations.

In this report a method for generating group constants for P_1 equations from evaluated data is outlined and the description of the related computer program is given.

2. Method for the calculation of group constants

The group constants are dependent on the equations in which they are to be used. For instance, a set of group constants prepared for S_n calculation is of doubtful applicability in diffusion calculation, and vice versa. Of course, if the energy mesh is small, i.e. the number of groups is large, then any set can be used for any purpose to a relatively good approximation. In the following only the calculation of group constants for P_1 approximation is considered; however, group constants for any other purposes could be obtained by similar consideration. The P_1 equations in their general energy dependent form are:

$$\forall J(r,E) + \Sigma(E)\phi(r,E) = \int dE' \Sigma_{O}(E' \rightarrow E)\phi(r,E') + \chi(E) \int dE' v(E') \Sigma_{f}(E')\phi(r,E') /2.1a/dE'$$

$$1/3 \nabla \phi(\mathbf{r}, \mathbf{E}) + \Sigma(\mathbf{E}) J(\mathbf{r}, \mathbf{E}) = \int d\mathbf{E}' \Sigma_{1}(\mathbf{E'} + \mathbf{E}) J(\mathbf{r}, \mathbf{E'})$$
 /2.1b/

Multigroup equations can be obtained on the assumption that there is space-energy separability in the i-th group as

$$\phi(\mathbf{r},\mathbf{E}) = \overline{\psi}(\mathbf{r}) \mathbf{f}(\mathbf{E})$$
 /2.2a/

$$J(r,E) = \bar{I}_{i}(r) j(E)$$
 /2.2b/

Inserting /2.2 into the Eqs./2.1/ and integrating for E over the interval (E_{i+1}, E_i) , we have

$$\nabla \mathbf{I}_{i}(\mathbf{r}) + \Sigma_{o}^{i} \psi_{i}(\mathbf{r}) = \sum_{k \neq i} \Sigma_{o}^{k \neq i} \psi_{k}(\mathbf{r}) + \chi_{i} \sum_{k} (\upsilon \Sigma_{f})^{k} \psi_{k}(\mathbf{r})$$
 /2.3a/

$$1/3\nabla\psi_{i}(r) + \Sigma_{1}^{i} I_{i}(r) = \sum_{k \neq i} \Sigma_{1}^{k+i} I_{k}(r)$$
 /2.3b/

$$\Sigma_{o}^{k-1} = \frac{\int_{E_{i+1}}^{E_{i}} dE \int_{C_{o}}^{E_{k}} dE' \mathcal{L}_{o}(E'+E) f(E')}{\int_{E_{k+1}}^{E_{k+1}} /2.4a/ \int_{E_{k+1}}^{E_{k}} dE f(E)}$$

$$\Sigma_{1}^{k+1} = \frac{\int_{i+1}^{E_{i}} dE \int_{k+1}^{E_{k}} dE' \Sigma_{1}(E'+E) j(E')}{\int_{E_{k+1}}^{E_{k}} dE j(E)}$$

/2.4b/

$$\left(\nu\Sigma_{f}\right)^{i} = \frac{\sum_{i=1}^{E_{i}} dE' \quad \nu(E') \quad \Sigma_{f}(E') \quad f(E')}{\sum_{i=1}^{E_{i}} dE \quad f(E)}$$

/2.4c/

$$x_{i} = \int_{E_{i+1}}^{E_{i}} dE \chi(E)$$
 /2.4d/

$$\Sigma_{o}^{i} = \Sigma_{tf}^{i} - \Sigma_{o}^{i+i}$$
 /2.4e/

$$\Sigma_{1}^{i} = \Sigma_{tj}^{i} - \Sigma_{1}^{i+i}$$
 /2.4f/



/2.4g/

$$\psi_{i}(r) = \overline{\psi}(r) \int_{E_{i+1}}^{E_{i}} dE f(E)$$

$$I_{i}(r) = \overline{I}_{i}(r) \int_{E_{i+1}}^{E_{i}} dE \ j(E)$$

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Over the thermal region, where there is no up-scattering, the equations become simpler. Namely, we may write $\begin{array}{c} i \ \Sigma \\ k=1 \end{array}$ instead of $\begin{array}{c} \Sigma \\ k\neq 1 \end{array}$, and

$$\Sigma_{0}^{i+i} = \frac{ \begin{array}{c} E_{i} & E & f(E') \\ \int dE & \int dE' & \Sigma_{0}(E' + E) j(E') \\ \hline E_{i+1} & E_{i+1} & 1 \\ \hline & \int dE & f(E) \\ & \int dE & j(E) \\ \hline & E_{i+1} \\ \end{array}}$$

In order to apply the above formulas, the energy spectra of flux and current, f(E) and j(E), should be known for every group. It is accepted that in the slowing-down region

$$f(E) = \frac{1}{E\Sigma(E)}$$
 /2.5a/

while in the thermal region

$$f(E) = -\frac{E}{T^2} e^{-E/T}$$
 /2.5a'/

where T is the material temperature.

The discussion here will be confined to the energy range above the thermal region. Group constants in this region will be calculated in accordance with other types of considerations, making use of the results of the theory of inelastic scattering in solid or liquid phase.

Between f(E) and j(E) there is an approximate relation

$$\mathbf{j}(\mathbf{E}) = \frac{\mathbf{f}(\mathbf{E})}{3\Sigma_{\pm \mathbf{r}}(\mathbf{E})}$$
 /2.5b/

where $\Sigma_{tr}(E)$ is the transport cross-section.

In the higher energy region there would be a better but more complicated option than /2.5a/, as

$$f(E) = \frac{E}{\Sigma(E) \Sigma E} + \chi(E)$$
 /2.5c/

 $/\chi$ (E) is the fission spectrum./

Generally, in the slowing-down region three types of nuclear processes lead to the energy degradation of neutrons: elastic $/\Sigma_{el}/$ and inelastic $/\Sigma_{in}/$ scattering and the /n,2n/ process $/\Sigma_{n,2n}/$. Thus

$$\Sigma_{o}(E' + E) = \Sigma_{el_{o}}(E' + E) + \Sigma_{in}(E' + E) + 2\Sigma_{n,2n}(E' + E)$$
 /2.6a/

$$\Sigma_1(E' \rightarrow E) = \Sigma_{el_1}(E' \rightarrow E)$$
 /2.6b/

It is assumed that the inelastic scattering and the /n, 2n/ process are isotropic in the laboratory system.

a/ <u>Elastic scattering</u>. Let $\sigma_s^{\ell}(E,\mu)$ be the differential elastic scattering cross-section in center-of-mass system, μ the cosine of scattering angle, M_l the mass of the nucleus, and Q_l the nuclear density, then /see [4]/

$$\int d\mathbf{u}' \Sigma_{el_0}(\mathbf{u}' + \mathbf{u}) f(\mathbf{u}') = \sum_{\ell} Q_{\ell} \frac{\left(M_{\ell} + 1\right)^2}{4M_{\ell}} \int_{\mathbf{u} - Q_{\ell}}^{\mathbf{u}} d\mathbf{u}' f(\mathbf{u}') \sigma_{\mathbf{s}}^{\ell} \left(\mathbf{u}', \mu(\mathbf{u}, \mathbf{u}')\right) e^{\mathbf{u}' - \mathbf{u}}$$

$$/2.7a/$$

$$\int d\mathbf{u}' \Sigma_{\mathbf{el}_{1}}(\mathbf{u}'+\mathbf{u}) \mathbf{j}(\mathbf{u}') = \sum_{\boldsymbol{\ell}} Q_{\boldsymbol{\ell}} \frac{\left(\mathbf{M}_{\boldsymbol{\ell}}+1\right)^{2}}{4\mathbf{M}_{\boldsymbol{\ell}}} \int_{\mathbf{u}-Q_{\boldsymbol{\ell}}}^{\boldsymbol{v}} d\mathbf{u}' \mathbf{j}(\mathbf{u}') \sigma_{\mathbf{g}}^{\boldsymbol{\ell}}(\mathbf{u}',\boldsymbol{\mu}(\mathbf{u},\mathbf{u}')) e^{\mathbf{u}'-\mathbf{u}}$$

$$\left[\frac{M_{\ell}+1}{2} - \frac{u-u'}{2} - \frac{M_{\ell}-1}{2} - \frac{u-u'}{2}\right]$$
 /2.7b/

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where

$$q_{\ell} = \ln \frac{(m_{\ell}+1)^2}{(M_{\ell}-1)^2}$$

and

$$\mu(u,u') = 1 - \frac{\left(\frac{M_{\ell}+1}{2}\right)^{2}}{2M_{\ell}} \left(1 - e^{u'-u}\right) \qquad (2.8)$$

In these the more convenient lethargy variable is used instead of energy variable, i.e.

 $u = \ln E_0/E$

Substituting /2.7/ into /2.4a-b/, we get

$$\Sigma_{el_{O}}^{k+i} = \sum_{\ell} Q_{\ell} \frac{\left(M_{\ell}+1\right)^{2}}{4M_{\ell}} \varepsilon_{ki}^{\ell} \int_{Y}^{u_{k+1}} du' f(u') \int_{w(u')}^{z(u)} \frac{du \sigma_{s}^{\ell}(u',\mu(u,u')) e^{u'-u}}{\int_{u_{k}}^{u_{k+1}} du f(u)}$$

$$\Sigma_{el_{1}}^{k+i} = \sum_{\ell} Q_{\ell} \frac{\left(M_{\ell}+1\right)^{2}}{4M_{\ell}} \varepsilon_{ki}^{\ell} \int_{Y}^{u_{k+1}} du' j(u') \int_{w(u')}^{z(u')} du \sigma_{s}^{\ell}(u', \mu(u, u')) e^{u'-u}$$

$$\left[\frac{M_{g}+1}{2}e^{-\frac{u-u'}{2}} - \frac{M_{g}-1}{2}e^{\frac{u-u'}{2}}\right] / \int_{u_{k}}^{u_{k+1}} du j(u)$$
 /2.9b/

$$\varepsilon_{ki} = \begin{cases} 1 & \text{if } u_i - u_{k+1} \leq q \\ 0 & \text{if } u_i - u_{k+1} > q \end{cases}$$
 /2.10a/

$$y = \begin{cases} u_{k} \text{ if } u_{i} - u_{k} < q \\ u_{i} - q \text{ if } u_{i} - u_{k} > q \end{cases}$$
 /2.10b/

$$z(u) = \begin{cases} u_{i+1} & u_{i+1} \leq q_{\ell} \\ u' + q_{\ell} & \text{otherwise} \end{cases}$$
 /2.10c/

$$w(u') = \begin{cases} u_{\underline{i}} & \text{if } \underline{i} \neq k \\ u' & \text{if } \underline{i} = k \end{cases}$$
 /2.10d/

If the integral variable u is changed to μ in /2.9/, then we have

$$\Sigma_{el_{0}}^{k+i} = \sum_{\ell} Q_{\ell} \frac{1}{2} \varepsilon_{ki}^{\ell} \int_{Y}^{u_{k+1}} du' f(u') \int_{\mu(z,u')}^{\mu(w,u')} d\mu \sigma_{g}^{\ell}(u',\mu) / \int_{u_{k}}^{u_{k+1}} du f(u) /2.11a/$$

$$\Sigma_{e1_{1}}^{k+i} = \sum_{\ell} Q_{\ell} \frac{|1}{|2} \varepsilon_{ki}^{\ell} \int_{Y}^{u_{k+1}} du' f(u') \int_{\mu(z,u')}^{\mu(v,u')} d\mu \sigma_{g}^{\ell}(u',\mu) \left[\frac{M_{\ell}+1}{2} \sqrt{1 - (1-\mu)} \frac{2M_{\ell}}{(M_{\ell}+1)^{2}} \right]$$

$$-\frac{M_{\ell}-1}{2}\left(\sqrt{1-(1-\mu)\frac{2M_{\ell}}{(M_{\ell}+1)^{2}}}\right)^{-1}\right] / \int_{u_{k}}^{u_{k}+1} du j(u)$$
 /2.11b/

If the scattering is isotropic in the center-of-mass system, i.e. $\sigma_s^{\ell}(u',\mu) = \sigma_s^{\ell}(u')$, then the inner integral in /2.11/ can be performed analytically, and we have

$$\Sigma_{el_{O}}^{k+i} = \sum_{\ell} Q_{\ell} \frac{(M_{\ell}+1)^{2}}{4M_{\ell}} \varepsilon_{ki}^{\ell} \int_{Y}^{u_{k+1}} du' f(u') \sigma_{s}^{\ell} \frac{(u') e^{u'}(e^{-u_{i}} - e^{-z(u')})}{u_{k+1}} /2.12a/2u_{k}$$

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$$\Sigma_{e1}^{k} = \sum_{\ell} Q_{\ell} \frac{(M_{\ell}+1)^{2}}{4M_{\ell}} \varepsilon_{k1}^{\ell} \int_{Y}^{u_{k}+1} du' f(u') \sigma_{s}^{\ell}(u') \left[\frac{M_{\ell}+1}{3} e^{3/2u'} \left(e^{-3/2} - e^{w(u') - 3/2(u')} \right) \right]$$

$$- (M_{\ell}-1) e^{-u'/2} \left(e^{-w(u')/2} - e^{-\frac{z(u')}{2}} \right) \right]$$
 /2.12b/

b/ Inelastic scattering. Inelastic scattering of neutrons is treated in one of two ways, depending upon the energy of the incident neutron, E'. Let E_c denote a target nucleus excitation energy below which the level structure of the nucleus is given. In the process of inelastic scattering, the incident neutron loses an amount of energy approximately equal to the energy of excitation of the residual nucleus, E_i , i.e. more precisely

$$\sigma_{\underline{i}n}^{\ell}(E' \rightarrow E) = \sum_{\underline{i}=1}^{C_{\ell}} \sigma_{\underline{i}}^{\ell}(E') \ \delta\left(E - \frac{M_{\ell}-1}{M_{\ell}+1}E' + \frac{M_{\ell}}{M_{\ell}+1}E_{\underline{i}}\right)$$
 /2.13/

/The sum is extended over the resolved excitation levels./

For $E' > E_c$ a continuous distribution, the so-called evaporation model, is used [5]:

$$\sigma_{\text{in}_{\text{cont}}}^{\ell}(\mathbf{E'} + \mathbf{E}) = \sigma_{\text{cont}}^{\ell}(\mathbf{E'}) \frac{\mathbf{E} e^{-\mathbf{E}/\Theta^{\ell}(\mathbf{E'})}}{\Theta^{\ell}(\mathbf{E'}) - e^{-\mathbf{E'}/\Theta^{\ell}(\mathbf{E})} (\Theta^{\ell}(\mathbf{E'}) + \mathbf{E'})} /2.14/$$

where

$$\Theta^{\ell}(E') = \sqrt{\frac{E'}{M_{\ell}}} / 0.31$$

*

Substituting /2.13/ and /2.14/ into /2.4a-b/, we obtain

$$\Sigma_{in}^{k,j} = \sum_{\ell} Q_{\ell} \left[\sum_{i=1}^{c_{\ell}} \int_{E_{k+1}}^{E_{k}} dE' f(E') \sigma_{i}(E') \varepsilon_{kj}^{i} + \sum_{i=1}^{k} \int_{E_{k+1}}^{E_{k+1}} dE' F(E') \sigma_{i}(E') \varepsilon_{i}^{i} + \sum_{i=1}^{k} \int_{E_{k+1}}$$

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$$\sum_{\substack{E_{k+1} \\ E_{k+1} \\ E_{k+1}$$

$$\int_{E_{k+1}}^{E_k} dE' f(E')$$

where

$$\varepsilon_{kj}' = \begin{cases} 1 & \text{if } E = \frac{M_{\ell} - 1}{M_{\ell} + 1} E' - \frac{M_{\ell}}{M_{\ell} + 1} E_{1} \text{ and } E \leq E' \leq E_{k} \text{ and } E_{j+1} \leq E \leq E'_{j} \\ 0 & \text{otherwise} \end{cases}$$

c/ <u>The [n,2n] process</u>. For the energy distribution of neutrons arising from the (n,2n) reaction the evaporation model is used, i.e. two neutrons are boiled off in succession with the mass number decreased by one for the second neutron.

$$2\Sigma_{n,2n}^{k+j} = \sum_{\substack{\substack{e \in \mathbb{Z} \\ q_{k} \\$$

where

$$\theta_1^{\ell}(E) = \sqrt{\frac{E}{M_{\ell}}} / 0.31$$

$$\theta_2^{\ell}(E) = \sqrt{\frac{E}{M_{\ell}-1}} / 0.31$$

3. The evaluated data file available at IAEA

The evaluated data file available at IAEA is composed from KEDAK and AWRE files. At the present it contains 13 files. Their content and other parameters are given in Table 1. The detailed description of the KEDAK and

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File	For- mat	Numb.of * char.in a block	Nuclei and types of data
1	AWRE	800	/n,γ/ cross-section for isotopes with mass number 83-160 /fission products/
2	KEDAK	800	For materials Al^{27} , C^{12} , Chromium, Iron, Deute- rium, H ¹ bound in H ₂ , H ¹ bound in H ₂ O, He ⁴ Mo, Na ²³ - all types of data required for group constant calculation; for isotopes of Chromium,
			Iron and Molybdenum resonance parameters only; for He ³ absorption and $/n,p/-cross-section$ only; for N ¹⁴ -differential elastic scattering only.
3	KEDAK	800	For Ni,0 ¹⁶ , Pu ²³⁹ , U ²³⁵ -all types of data needed for group constant calculation; for isotopes of Ni-resonance parameters only.
4	KEDAK	800	For Cd, Pu ²⁴⁰ , Pu ²⁴¹ , Pu ²⁴² , U ²³⁵ -all types of data needed for group constant calculation.
5	AWRE	800	For Zr-all types of data needed for group constant calculation.
6	AWRE	800 •	For Th ²³² -all types of data needed for group constant calculation.
7	AWRE	800	For Be, Pu ²⁴¹ , B ¹¹ -all types of data needed for group constant calculation.
8	AWRE	800	Pu ²³⁹ - all types of data needed for group constant calculation.
9	AWRE	800	For U ²³⁵ - all types of data needed for group constant calculation.
10	AWRE	800	For U ²³⁸ - all types of data needed for group constant calculation.
11	AWRE	800	$/n,\gamma/$ cross-section for isotopes with mass number 81-157 /fission products/.
12	AWRE	80	For Li ⁶ - all types of data needed for group constant calculation.
13	AWRE	80	For Li ⁷ - all types of data needed for group constant calculation.

AWRE format can be found in the reports [6] and [7], respectively. Here we restrict ourselves to the main features of these formats, discussing the essential differences between them.

a/ KEDAK format

At the beginning of each KEDAK file there is a description of material contents. At the beginning of data group for each material there is a description of data type contents.

The information is arranged in records of 80 characters /cardimage format/. The 73-80 character positions are the identification part of the record.

73-74 are the positions at which the material appears in the description of the material contents,

75-76 are the positions at which the data type appears in the description of the data type contents,

77-80 are the serial number of the card in the given data group.

Before each data group there is a record containing the number of data sets in that group. If there are further parameters /e.g. energy of excitation level at inelastic scattering, or incident neutron energy for differential scattering cross-section, etc./, then they are given in a record before that containing the number of data sets. Each data group begins with the information on the material type, data type, number of further parameters, number of arguments and functional values, and number of different values of further parameters.

b/ AWRE format

One of the most essential and disconcerting differences between the KEDAK and AWRE format is in the identification of nuclei. In the AWRE files the data sets of a given material are identified with a number of three figures which is arbitrary chosen by the editors of the file. This number is placed in the 73-75 character positions of each record. The numbers placed in the 73-76 character positions of any KEDAK file are nondescending, and this is not true for AWRE files.

The identification of data groups for a given material is similar to that in KEDAK files, the only difference being that the 76-77 character positions serve for this purpose.

The energy range covered is divided into some particular intervals. Before the data group for each interval there can be found information on the lower and upper limit of the interval, the material temperature, the number of data sets in this interval, and the number of temperatures still to be fully considered. Thus the number of data sets in the local energy range can not be recognized at once before the data group. This is also an uncomfortable feature of AWRE files.

There are differences not only in the form of the files but in their content too. Transport cross-sections are generally missing in the AWRE files. While in KEDAK files the differential elastic cross-sections are given, in AWRE files only the probability of angular distribution can be found /and, of course, the total scattering cross-section/. While in the KEDAK files the energy of excitation level is a further parameter, in the AWRE files the inelastic cross-sections for every excitation level are represented by separate data groups.

A great effort has been made in order to confine the effect of differences in data source on the structure of the program processing these data. This problem will be discussed in detail in the next section.

4. Stages of the production of multigroup constants

There are three stages in the calculation of multigroup constants from the evaluated data files. In any stage the calculation starts from a • magnetic tape data file and the work is finished with a newly created magnetic tape data file. Each file has a specific and strictly defined structure characterizing the job performed in the stage. The evaluated file originating from IAEA will be denoted by DFO. The files created by the three stages are denoted by DF1, DF2, DF3, respectively.

While the file DFO is written by the special magnetic tape-handling subroutines for the ICL-1905 computer, the files DF1, DF2 and DF3 are written by the ICL standard FORTRAN system.

1st stage

The program searches the data groups of any given material and searches the data type for this material. The position of the data, i.e. characters 73-76 /for AWRE data 74-77/ of the data cards, should be specified by input paper tape. Data are read in, converted into binary form and written on to DF1 in a rearranged order.

For any material on the file DFl there are at most 15 data types in a strictly definite order, as shown in Table 3. The structure and format of DFl are given in Table 2.

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Table 2.

Information type	List of I/O statement	Content
Introduc- tory	KE/I/,NFU/I/,I=1,50	KE/I/, for I=-48, the name of materials contained in DF1; KE/49/, number of materials KE/50/, number of data types /15/ NFU/I/= n_i , where if $n_i=0$ or -2 then the i-th material is non-fissionable; if $n_i = 1$ the i-th material is fissionable; if $n_i = 0$ the i-th material is on an AWRE file, otherwise it is on a KEDAK file.
Records for a given mate- rial and da- ta type, and, if there is a further parameter, then for a	KR/I/ I=1,6 *	<pre>KR(1)=K₁, number of data sets KR(2)=K₂, number of data records KR(3)=K₃, number of further pa- rameters KR(4)=K₄, number of arguments KR(5)=K₅, number of functional values KR(6)=K₆, number of combinations of further parameters</pre>
given value of it	FN/I/, I=1,3	This record exists if K ₃ =0 FN(1) = the value of the further parameter; FN(2) = atomic mass of the mate- rial /only for AWRE data/
	NKR, AC/J/,DC/J/=1, NKR	NKR < 2250 AC/J/argument, DC/J/functional value K ₂
	IBS	Number of record for this data type

a given ma- terial rial type	A record for IE a given ma- terial	BN .	Number of re rial type	ecord for	this mate-
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^xIf for a given data type the given material does not exist or is zero then $K_1 = 0$ and the records except the first and the last one are omitted.

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Table 3.

No.	Name	Description and remarks
1	SGT3	total cross-section
2	STR3	transport cross-section in KEDAK, total cross- section in AWRE files
3	SGN3	elastic scattering cross-section
4	SGI3	total inelastic scattering cross-section
5	S2N3	cross-section for the /n,2n/ process
6	SGA3	absorption cross-section
7	SGG3	cross-section for $/n,\gamma/$ process
8	SAL3	cross-section for /n,a/ process
9	SGX3	nonelastic cross-section
10	SPR3	cross-section for /n,p/ process
11	SGE3	inelastic cross-section for excitation of rest nucleus level E _i
12	SNC4	differential elastic scattering cross-section in the center-of-mass system in KEDAK, and scatter- ing probability in AWRE files
13	SGF3	fission cross-section
14	NUE3	average number of fission neútrons.
15	КНРЗ	energy spectrum of prompt fission neutrons

<u>Remarks</u>: 1/ except for SNC4, the argument is the neutron incident energy;

- $2/E_{i}$ is a further parameter for SGE3;
- 3/ The neutron incident energy is a further parameter for SNC4.

It should be mentioned that because of the restricted fast memory capacity, there can be at most 2250 pairs of data in a record. The number of records for a given data type is indicated by K_2 .

The differences between the KEDAK and AWRE data are much less on DF1 than on DF0. All differences vanish on DF2, i.e. at the end of second stage.

2nd stage

In this stage an energy argument system is introduced /EAS/ which is uniform for any materials and for any types of cross-section that are to be compiled together. The term "compiled together" will be clarified later. The total energy range in question /generally O-10 MeV/ is divided into N intervals. This division will correspond to the multigroup system to be constructed. The intervals are divided into subintervals, i.e. a fine group system is introduced. The middle points of the fine group intervals constitute the above-mentioned EAS. The number of fine groups in a broad group may be quite large ≤ 200 , thus allowing the fine structure of the cross-section to be followed.

The serial number of materials on DF1 to be compiled together on DF2 are specified by input. First the data of these material are scanned and copied on a scratchtapes while the record number of each data group is put down in a matrix. This matrix controls the data search on the type which has been copied from DF1.

The data are interpolated and written on the DF2 which is prepared in this stage. Above 1 eV the interpolation of data is performed linearly in lethargy, below 1 eV this is done linearly in energy.

The structure of DF2 is shown in Table 4. and it clarifies what we mean by the term "compilation". The DF2 file is organized so that the macroconstants of any mixture containing only the materials compiled together can easily be calculated in the next stage. Thus DF2 may be regarded as a generalized microgroup constant set which can be flexibly used for any purpose.

It should be mentioned that at the cost of some additional calculations all differences in KEDAK and AWRE data are eliminated.

3rd stage

In this stage macrogroup constants are produced by means of the formalism presented in the 2^{nd} section. The calculated macroconstants are written on DF3. In a run we may calculate as many mixtures as we wish. The composition of the mixture is specified by input from tape.

The application of the formalism presented in Section 2 requires the determination of the flux and current and numerical integration over the group intervals. The flux and current are calculated by Eqs. /2.5/, and the numerical integrations are performed by a simple trapezoidal rule.

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Informa- tion type	List of I/O statement	Content
lntroduc- toiy	NDM,NG,NE,NF, /KFZ/I/,NF2/I/,I=1,NE/ /M/I/, I=1,NG/, /UG/I/, I=1, NG+1/	<pre>NDM=the number of data type/15/ NG=number of broad group NE=number of materials NF=1 if the material is fis- sionable, NF=0 otherwise KFZ/I/ = KE/I/ NFZ/I/ = NFU/I/ M/I/=number of fine groups in the i-th broad group UG/I/=the upper boundary of the i-th broad group/in eV/</pre>

For the j-th data type j=l - 10	k-th mate- rial	i-th broad group	ST/L/,L = 1,M/I/	values of the j-th data for k-th material, for the energy values EAS inside the i-th broad group
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For the	k-th				
11 th	mate-	i-th			
data type	rial	broad group	j-th energy values of EAS inside the i-th group	N,/E/L/, S/L/,L= 1,60/	N is the number of E/L/excitation energy values; S/L/is the corresponding inelas- tic cross-section
		,			
		i-tho broad group	ST/L/,L=1,M/	I/ tota sect	al inelastic cross- tion

12 ^{ch} data type	k-th mate-	i-th broad	group	ST/L	/,L=1,M/I/	elastic cross-section
type	rial	(1_+h				
		broad	j-th value	energy s of	ANU/L/,ASU	/L/, Angular values and values of corres-
		group	EAS in the i	nside -th	L=1,21/	ponding differenti- al elastic cross-

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k-th mate-	13th ype	1-th broad group	ST/L/,L≈l,M/I/	fission cross- section
rial	14th type	1-th broad group	ST/L/,L=l,M/I/	average number of neutron per fission
1sth	No.4h			
data type	mate- rial	1-th broad group	ST/L/,L=1,M/L/	fission spectrum

Table 5.

Information type	List of I/O statements	Content
Introduc- tory	NE,NG,NF,JLO,KE I AM I,RO I,I=1,NE	NE is the number of materi- als in the mixture; NG is the number of broad groups; NF=1 for fissionable mix- ture, NF=0 otherwise; JLO is the maximum group chan- ge in a collision; KE means the name of the materials, AM is its atomic mass, and RO is the nuclear density.
i-th group	/CRO/J/,CRT/J/,J=l,`ʔ/, /TRAN/J/,TRANI/J/J=I,NG/, SF, SNF, HAS/I/	CRO/J/ and CRT/J/ are macro- cross-sections for data type j=1-10 averaged over the flux and current, respectiv- ely; TRAN/J/ and TRANI/J/ are transfer cross-sections; SF is the fission macro- cross-section; SNF is the average number of neutrons per fission; HAS/I/ is the fission spectrum.

5. Description of the functions and subroatines of the program

Corresponding to the three stages discussed in the previous section, there are three main subroutines: DATFIL, CONSTP1 and GROUP. Another three subroutines CONTROL, OUTLIST, EDITOR respectively check the results of their work

DATFIL

DFO and DF1 are opened in DATFIL, and the job concerning the first stage is performed by means of the following related subroutines:

ARED- reads the next record of 80 characters on DFO and places them in an array which serves as an input periphery

FINDELEM- searches the first record of a given material on DFO

FINDKEDAK - searches the first record of a given data type for the material in question /data must be in KEDAK format/

FINDAWRE - does the same job as FINDKEDAK but for data in AWRE format

DARE - converts and rearranges the data which are in KEDAK format and edits the DF1

AWDARE - does the same job as DARE but for data in AWRE format

CONTROL

This procedure performs a checking output for a given material and given data type on DF1.

CONSTP1

DF2 is opened in CONSTP1 and the job concerning the second stage is performed by means of the following related subroutines and functions:

HELYMEG - puts down the place number of data records to be searched on the scratch tape prepared by copying DF1

TOLTELEM - copies the data from DFl on to a scratch tape

FORELEM - scans the data groups on DF1

energy.

SIG /function/ - calculates the cross-section on the energy points of EAS by averaging over the fine group interval

BSIG /function/ - supplies any cross-section value at a given energy point by interpolating data values on DF1

SEARCH - searches a given data type for a given material on DFl

CINT /function/ - performs the interpolation in energy

OLV - reads the arguments and cross-section values from DF1

ESIG - supplies the inelastic cross-section at a given energy point for all excitation level lower than this energy

SITRAN - calculates the transport cross-section in the case of AWRE data NUSIG - supplies the differential elastic scattering cross-section at a given

OUTLIST

This subroutine performs a checking output for a given data type of all materials on DF2.

GROUP

DF3 is opened in GROUP and the job concerning the third stage is performed by means of the following related functions and subroutines: MIXOLV - reads in the cross-section data for a given group for all materials

and produces the macro cross-sections for all energy points inside the group

- 18 -

FLUXUS - calculates f(E) and j(E) for all energy points inside the group, making use of $\Sigma_{tot}(E)$ and $\Sigma_{tr}(E)$ calculated by MIXOLV

SINT - performs the numerical integration by trapezoidal rule

IRG /function/ -supplies the sorial number of that group to which a given energy value belongs

ASPN /function/ - interpolates the differential scattering cross-section by angular variable

DIV - calculates the energy distribution by the evaporation model.

EDITOR

This subroutine performs a checking output of all macrogroup constants for a given group.

The connections between the subroutines and functions are shown in the block diagram /Fig. 1./. Koman numbers indicate the overlay structure of the program; i.e. subroutines with the same Roman number are in the same layer.

6. Versions for program operations and the description of the input

By use of a switch number any of the stages can be operated separately if the corresponding input DF is available /e.g. it has been prepared in an earlier run/. Thus, for instance, if we have a library of type DF2 for a given set of materials, the group constants of any mixture consisting of some of these materials can be calculated immediately by operating the third stage only.

The input paper tape is described by stages. The input format is a free one, that is the items are separated by two spaces; only the number of items in a line is restricted.

Input for the 1st stage

prepared

LINE FORMAT VARIABLES DESCRIPTION 1 IO KN Number of materials on DF1 to be



Fig. 1

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LINE	FORMAT	VARIABLES	DESCRIPTION
2	A4,2X,A8,IO	KE(I),SNE [*] (I), NFU(I)	KE(I) is the name of the material /in four characters/. SNE(I): the last two characters give the name of the subfile in which the given material can be found on DFO; the 3^{rd} character is 2 for KEDAK files, 3 for AWRE ones; 4^{th} and 5^{th} characters are arbit- rary; characters 6-7 or 6-8 are the identification number of material. NFU(I) is n_i /see Table 2.!
3	5(A4,2X)	NK [×] (J)	Data type identification numbers

Only for AWRE data:

LINE	FORMAT	VARIABLES	DESCRIPTION
4	IO,10 2X,A4	KR(6),NK(I+20), I=1,KR(6)	KF(6) is the number of inelastic scattering levels. NK(I+20)are the identifications of data for these
		,	levels.

Remarks: 1/ Lines 3 and 4 are repeated for each material.

2/ If a data type for a material does not exist or is zero, then the last two characters of NK(J) should be OO.

Input for CONTROL

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IE,JX,JD(I),I=1,JX IE = the serial number of material on DF1 to be checked: JX is the number of data types; JD(I) is the serial number of data to be printed out.

Remarks: 1/ IE and JX should be given in a strictly increasing order 2/ If IE=0 then the work of CONTROL is terminated.

X Characters for SNE and NK can be found in Table 6.

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Input for 2nd stage

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LINE	FORMAT	VARIABLES	DESCRIPTION
1	210,F0.0	NG,NU,T	NG is the number of broad group : if NU=0, then the broad group boun- daries are the same as for the Abagyan set [2]; if NU=0, then they should be specified by input. T is the temperature
2	1010	M/I/,I=1,NG	Number of fine groups in the broad groups
3	10F0.0	UG/1/,1=1,NG	Broad group boundaries /this line is present unless NU=0/
4	310	NIS,NF,NE	NIS=0 if there are not more groups of materials to be compiled to- gether, NIS=0 otherwise; if there are fissionable materials among those to be compiled then NF=0, otherwise NF=0; NE is the number of materials.
5	1010	NTM/I/,I=1,NE	The serial number of material on DFl
		Input of OU	TLIST
1	1010 J	D,NX,JGX/I/,I=1,NX	JD is the data type number; NK is the number of broad groups for which fine group cross-section of JD data type are to be printed out. JGX(I)are the broad group indices
Remarks	: 1/ JD and	JGX should be given	in a strictly increasing order,
	2/if NX if (NX)	=0 but JD=0, then th =JD=0, then the job	e next compilation is taken; of OUTLIST is terminated.
		Input for t	he 3 rd stage
1	F0.0,210	T,NF,NE1,JLO	T is temperature; NF has the same meaning as in the 2^{nd} stage; NE1 the number of material in the mixture; JLO is the maximum group change by a scattering /at present this is $\leq 10/$

LINE	FORMAT	VARIABLES	DESCRIPTION
2	A4,2F0.0	KFZ(I),AMZ(I),RZ(I), I=1,NE1	KFZ = material name AMZ = atomic mass RZ = nuclear density
3	10	J	J=0 if no further mixture to be calculated, J=0 otherwise.
		Input for E	DITOR
1	10	IG	IG is the broad group index for which the transfer cross-section should be printed

if IG=O, EDITOR is terminated if IG=O, the cross-sections are punched out.

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					_	data.	AWRE	s for	evels	ion]	citat	ice ex	istan	ford	ring	scatte	elastic	X = Iné
400	47	411	416	414	400	419	400	412	410	416	413	415	418	417	4	EI24	KEDAK	PU42
0016	0017	0014	00 3	0000	0000	00 4	0000	0018	0000	00 8	00 00	00 2	100	00 1	60	EN33	AWRE	PU41
300	3 7	311	316	314	300	319	300	312	310	316	313	315	318	317	m	EI24	KEDAK	PU41
200	2 7	211	216	214	200	219	200	212	210	216	213	215	218	217		EI24	KEDAK	PU4
0030	0031	0028	т 00	00 5	0000	00 4	0000	0032	0000	0022	0019	00 7	00 1	00	065	EF33	AWRE	PU39 ^X
с С	80 80	813	818	816	819	822	812	814	811	823	815	817	821	820	œ	EH24	KEDAK	PU39
0046	0047	0044	о 00	00 00	0000	00 4	0000	0048	0000	0038	0035	00 7	00	8 8	401	ER33	AWRE	U238 [*]
5 2	5 6	511	516	514	517	520	510	512	5 0	521	513	515	519	518	ŝ	EI24	KEDAK	U238
0034	0035	0032	00 00	00	0000	00 4	0000	0036	0000	0026	0023	00 2	00 00	00 1	066	EQ33	AWRE	U235 [×]
ი ი	6 8	913	918	916	616	922	912	914	116	923	915	917	921	920	6	EH24	KEDAK	U235
0000	0000	0000	о 00	0000	0000	00 4	0000	0018	0000	80 00	00 5	00 2	00 1	00 1	22	EM33	AWRE	TH32
1800	1800	1800	1812	1810	1813	1816	18 7	18 8	18 6	1817	18 9	1811	1815	1814	18	EG24	KEDAK	M000
100	100	100	100	1 8	110	113	100	г 6	14	114	. 1 7	ი ი	112	111	Ч	EI24	KEDAK	CDOO
0000	0000	0000	00 3	0000	0000	00	0000	0000	0011	80	00 5	00 2	80 1	ы 1	6	EK33	AWRE	ZR91
100	100	100	112	110	113	116	17	1	1 6	117	1 9	111	115	114	Ч	EH24	KEDAK	00IN
800	800	800	812	810	813	816	87	80	8 8	817	80 6	811	815	814	00	EG24	KEDAK	FEOO
300	300	300	312	310	313	316	3 7	80 M	9 M	317	6 M	311	315	314	m	EG24	KEDAK	CROM
100	100	100	111	Г Р	112	115	1	17	1 1	116	1	110	114	113	н	EG24	KEDAK	AL27
2700	2700	2700	2711	27 9	2712	2715	27 6	27 7	27 5	2716	27 8	2710	2714	2713	27	EG24	KEDAK	NA23
700	700	700	711	7 9	712	715	76	77	75	716	7 8	710	714	713	~	EH24	KEDAK	0-16
200	200	200	211	2 9	212	215	2 6	2 7	2 5	216	8 8	210	214	213	2	EG24	KEDAK	C-12
0000	0000	0000	0000	00 4	0014	0000	0016	0013	0000	0000	0010	00	00	00 1	49	EN33	AWRE	B-11 ^X
0000	0000	0000	00 3	0000	00 6	00 4	0010	8 0 0	0000	00 5	0000	8	00	00 1	50	EN33	AWRE	BE-3
0000	0000	0000	00 00	00 00	0000	00 4	0017	0016	0000	00 7	0013	00	00 1	00 1	215	1233	AWRE	LI-7
0000	0000	0000	00 00	00 00	0014	00 4	0015	0013	0000	0010	0000	00 2	00 1	-1 00	214	1133	AWRE	D-11
1700	1700	1700	17 9	1700	1710	1713	17 5	17 6	17 4	1714	17 7	17 8	1712	1711	17	EG24	KEDAK	HE-4
1300	1300	1300	13 9	1300	1310	1313	13 5	13 6	13 4	1314	13 7	13 8	1312	IIII	1 13	EG24	KEDAK	DE-2
1500	1500	1500	1500	1500	15 7	1510	15 3	15 4	15 2	1511	15 5	15 6	15 9	158	1 15	EG24	KEDAK	H20B
1400	1400	1400	1400	1400	14 7	1410	14 3	14 4	14 2	1411	14 5	14 6	14 9	14 8	1 14	EG24	KEDAK	H-1B
KIP 3	NUE4	SGF 3	SNC4	SGE3	SPR3	SGX3	SAL3	SGG3	SGA3	S2N3	SGI3	SGN3	STR3	SGT3	E	SN	Format	Material name

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Tab	le	6	b	•
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Material name	Number of levels	2	3	4	5	6	7	8	8	lo
B-11 U235 U238 PU	3 6 10 7	00 6 00 8 00 8 00 7	00 8 0011 0011 00 9	0014 0014 0011	0017 0017 0013	0020 0020 0015	0023 0017	0026	0029	0032

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