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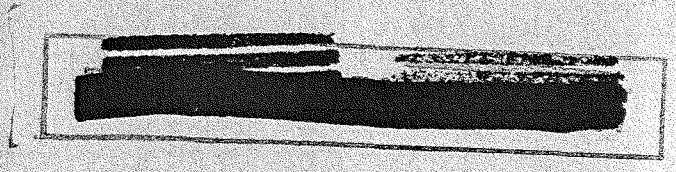
O.E.C.D. HIGH TEMPERATURE REACTOR PROJECT

DRAGON

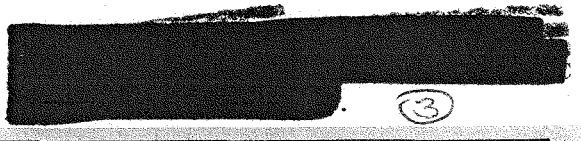
Dragon Project Report



MUPO
AN IBM—7090 PROGRAMME TO CALCULATE NEUTRON SPECTRA AND MULTI-GROUP CONSTANTS

by

J. SCHLÖSSER



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MUPO, AN IBM-7090 DIFFUSION PROGRAMME TO CALCULATE NEUTRON SPECTRA AND MULTI-GROUP CONSTANTS

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ABSTRACT

MUPO calculates the zero dimensional neutron spectrum in 43 energy groups. This spectrum is used to evaluate condensed microscopic and macroscopic cross sections for various other programmes.

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MUPO, AN IBM-7090 DIFFUSION PROGRAMME TO CALCULATE NEUTRON SPECTRA AND MULTI-GROUP CONSTANTS

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1. INTRODUCTION

The Reactor Physics Group of the Dragon Project used until recently as basic programme for calculating the neutron spectrum and group cross sections the STEWPOT programme. It was written by M. J. Brinkworth, R. J. Brissendon and C. P. Gratton of the United Kingdom Atomic Energy Authority, for the Mercury Ferranti Computer and was reported upon by L. Massimo and E. Schröder [1] of the Dragon Project. In the meantime a larger computer (IBM-7090) became available and it was thought desirable to use its greater capacity and speed by writing a programme, more flexible, faster and easier to operate than STEWPOT. A detailed description of it is given in this paper.

MUPO solves the zero dimensional diffusion equation in 43 energy groups, whereby the user has the choice between three options of calculating the neutron spectrum: by introducing an additional absorber to account for a control poison, by a source iteration technique and by a buckling iteration as in STEWPOT. Additionally, the programme accepts as input either 43 group fluxes or 18 group fluxes for the evaluation by interpolation of 43 group fluxes. Having obtained the neutron spectrum the programme proceeds to calculate a condensed absorption - and fission - matrix and microscopic cross sections for all isotopes specified. Several options are included in the programme for punching group cross sections on cards which can be directly used by a number of one and two-dimensional diffusion programmes.

2. DESCRIPTION OF THE PROGRAMME

The programme is best described by means of the flow diagram, Fig. 1. All nuclear data, cross sections, resonance tables and scattering matrices are provided on magnetic tape. These may be completely printed by the programme itself. In any case the user obtains a summary of the content of the library - especially identification numbers of the isotopes and temperature of the scattering kernels available - prior to any calculation. Furthermore the programme is able to generate its own library tape by reading the necessary data from cards (see Sections 2.5 and 3.5). After that, parts of the input data are read and the tape searched for the cross sections of the isotopes wanted. As the transport and absorption cross sections of the resonance materials take only the $1/v$ part into account, the resonance part has to be added. It is given in the form of two parametric tables, (see Section 2.5). The cross sections are then modified to account for flux depression by means of disadvantage factors which are part of the input. These cross sections together with the corresponding concentrations are printed by the programme. After completion the tape is scanned for the scattering kernel with the temperature wanted and the 43 x 43 macroscopic absorption and fission matrices assembled. At this point several options of calculating the neutron spectrum are available to the user. They are described in the following paragraphs.

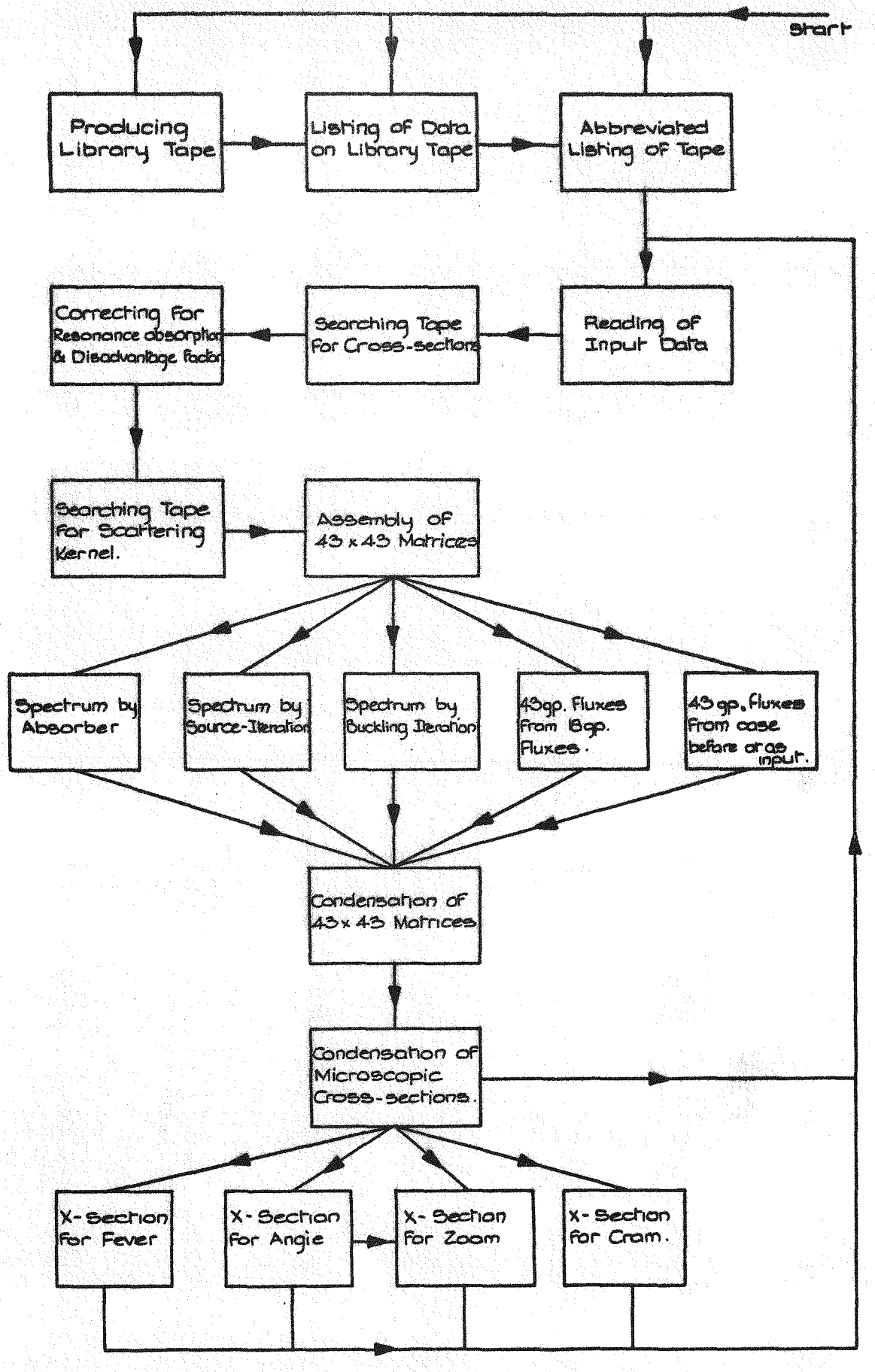

FIG. 1 FLOW DIAGRAM OF MUPO.

2.1 The Calculation of the Neutron Spectrum

To arrive at the equations solved by the programme let us consider the general zero-dimensional diffusion equation in 43 energy groups (index j):

$$\varepsilon B_j^2 D_j \phi_j + \Sigma_{tj} \phi_j + c_o \sigma'_{aj} \Phi_j \qquad (1)$$

$$- \left(\text{Sum}_{i=1}^{43}\right) \left\{\frac{\nu}{k_{eff}} y_j \Sigma_{fi} \phi_i\right\} - \left(\text{Sum}_{\substack{i=1 \\ i\neq j}}^{43}\right) \left\{\Sigma_{sc} (i \longrightarrow j) \phi_i\right\} = 0$$

$$j = 1, 43$$

where B_j^2 is the energy dependent buckling term

Σ_{aj} the macroscopic absorption cross section

Σ_{tj} the macroscopic total cross section (capture plus fission plus scattering out)

σ'_{aj} the microscopic absorption cross section of an additional absorber, symbolising a control poison

D_j the macroscopic diffusion coefficient

$\nu\Sigma_{fj}$ the total macroscopic neutron production cross section

$\Sigma_{sc}(i \longrightarrow j)$ the macroscopic transfer cross section from group i to j

y_j the relative number of fission neutrons entering group j

ε, c_o, k_{eff} are parameters used to make the determinant of the system vanish.

To make the programme suitable for the various requirements of neutronic calculations three parameters ε, c_o, k_{eff} are introduced in the above system of equations. They represent the three options, available to the user, for evaluating the neutron spectrum.

Case 1 the programme calculates c_o for $k_{eff} = 1$ and $\varepsilon = 0$. This option is suited best for evaluating the spectrum and group cross sections for burn-up calculations in a large reactor, where the loss of neutrons by leakage is negligible and the neutron spectrum is strongly influenced by the presence of control rods in the core. The programme reads as input the microscopic absorption cross sections of the control poison in 43 energy groups already multiplied by the proper self-shielding factors and calculates the critical concentrations c_o for which the determinant of the system (1) is zero, or in other words, the infinite homogeneous reactor is critical.

Case 2 the programme calculates k_{eff} for $c_o = 0$ and $\varepsilon = 1$. This is the so

called source iteration process, because the production of fast neutrons is changed by varying k_{eff} until the determinant of the system (1) vanishes. To account for loss of neutrons by leakage energy-dependent buckling terms are accepted. This option is particularly useful in evaluating the spectrum of small reactors, or in volume elements in a reactor with changing isotope composition. The possibility of introducing energy-dependent leak-rates which can be calculated using one and two-dimensional diffusion programmes like ZOOM [2], ANGIE [3] DDB [4] greatly improves the accuracy of the calculated neutron spectrum [5].

Case 3 the programme calculates the geometrical buckling εB^2 of the specified isotope concentration by putting $k_{eff} = 1$, and $c_o = 0$. Naturally, the buckling is the same for all energy-groups. This type of calculation is equivalent to the method used in STEWPOT [1]. It seems to be particularly useful for calculations on exponential stacks.

Spectrum calculations and the evaluating of group cross sections are calculations frequently carried out in modern reactor analysis. Besides this, the programme is being linked with the one-dimensional few-group burn-up programme FEVER [6], so that the few-group microscopic cross sections used for calculating the burn-up are re-evaluated from time to time to account for spectrum changes due to the depletion and build-up of fertile, fissile and poisonous isotopes. Furthermore, it is thought to use the programme as a sub-routine for obtaining the flux spectrum in a zero-dimensional multi-group burn-up code. Great care was therefore taken in speeding up the solution of the problem as much as possible.

In order to avoid solving the complete 43 x 43 matrix certain restrictions are imposed on the fairly general equations system (1). It seems to be a reasonable simplification to neglect the influence of inelastic scattering on the neutron spectrum of graphite moderated thermal reactors. Furthermore, fast and epithermal neutrons, scattered elastically on graphite suffer only a maximum energy loss of 0.334 in lethargy units. Therefore, scattering only into the next lower group is taken into account which requires that energy groups are wider than the equivalent of 0.334 lethargy units. This, however, is not a severe restriction because the total energy band to cover is some 21.5 units of lethargy wide, so that the spacing of energy boundaries is on average $\Delta u = 0.5$.

In the thermal region neutron scattering is influenced by the thermal oscillations of the moderator atoms and neutrons can lose and gain energy larger than the equivalent to $\Delta u_o = 0.334$. Therefore, the programme allows arbitrary up and down-scattering within the first 24 energy-groups.

Another restriction is imposed on the total width of the nine highest energy groups. Only these nine groups have source terms for fission neutrons. With an average energy-spacing of 0.5 lethargy units, however, only 1% of all fission neutrons from U-235 fall outside this range. One will in fact choose a larger spacing in order to obtain smaller groups in the more important thermal range, therefore altering the fission source distribution much less.

With these limitations the equations system (1) can be written as:-

$$\varepsilon B_j^2 D_j \phi_j + \Sigma_{aj} \phi_j + c_o \sigma'_{aj} \phi_j + \left(\text{Sum}\right)_{\substack{i=1 \\ i\neq j}}^{24} \left\{\Sigma_{sc} (j \longrightarrow i) \phi_j\right\} \qquad (2)$$

$$= \left(\text{Sum}\right)_{\substack{i=1 \\ i\neq j}}^{25} \left\{\Sigma_{sc} (i \longrightarrow j) \phi_i\right\} \qquad j = 1, 24$$

$$\varepsilon B_j^2 D_j \phi_j + \Sigma_{aj} \phi_j + c_o \sigma'_{aj} \phi_j + \Sigma_{sc} (j \longrightarrow j-1) \phi_j \qquad (3)$$

$$= \Sigma_{sc} (j+1 \longrightarrow j) \phi_{j+1} \qquad j = 25, 34$$

$$\varepsilon B_j^2 D_j \phi_j + \Sigma_{aj} \phi_j + c_o \sigma'_{aj} \phi_j + \Sigma_{sc} (j \longrightarrow j-1) \phi_j \qquad (4)$$

$$= \left(\text{Sum}\right)_{i=1}^{43} \left\{ \frac{\nu}{k_{eff}} y_j \Sigma_{fi} \phi_i \right\} = \Sigma_{sc} (j+1 \longrightarrow j) \phi_{j+1}$$

$$j = 35, 43$$

The method used to solve these equations is described for the source iteration routine; the other routines follow a similar scheme. Firstly, the equations (2) are solved using an iterative version of Crout's reduction (see for instance [7]). The group flux $\phi(25)$ being normalised to one gives the source term for the thermal region. The original 24 x 24 matrix containing the scattering, absorption, and buckling terms is reduced to a triangular matrix which is then solved starting with $\phi(24)$ down to $\phi(1)$.

The epithermal fluxes ($\phi(26)$ to $\phi(35)$) are readily calculated by applying equation (3), so that the thermal and epithermal neutron production is known. The last nine equations for the fluxes $\phi(35)$ to $\phi(43)$ (equation (4)) are solved by an iteration process which converges rapidly because the number of thermal and epithermal source neutrons exceeds by far those produced in the fast region. Normally three sweeps are sufficient to reduce the relative change in the fluxes in consecutive iterations to 10^{-5}. A comparison is then made between the group flux $\phi(35)$ calculated previously by equation (3) and the flux for the same group, $\phi'(35)$ calculated using equation (4). k_{eff} is altered according to

$$k_{eff}^{i+1} = k_{eff}^{i} \frac{\phi'(35)}{\phi(35)} \qquad (5)$$

until the relative change in k is smaller than 10^{-5} in consecutive iterations. Again, experience has shown that three iterations on k_{eff} are sufficient to fulfil the required accuracy.

The procedure used for calculating the spectrum by adjusting the control poison (Case 1) or the buckling (Case 3) is essentially the same. The difference is only that instead of k_{eff} (equation (5)) the control poison concentration or the buckling is altered according to a linear interpolation which uses the flux ratio $\left(\frac{\phi'(35)}{\phi(35)}\right)$ of consecutive iterations. It is obvious that both routines are slower than the source iteration process because all 43 fluxes have to be recalculated after every adjustment of the buckling or the control poison concentration whereas in the case of the source iteration routine only the nine fastest group fluxes are to be recalculated.

Having calculated the 43 group fluxes the programme renormalises them so that the sum is equal to one hundred. This seems to be a better way of normalising than fixing the value of one group flux. The programme proceeds then to evaluate broad group fluxes and broad group cross sections for the various applications (see Section 2.4).

2.2 Some Remarks on Reflector Spectrum Calculation

The three methods described until now for evaluating a neutron spectrum require the presence of a fission source. They fail when fluxes in a reflector region are to be calculated. To overcome this difficulty one can add to the isotope concentrations of the reflector a very small amount of a fissile material, e.g. 10^{+15} U-235 atoms per cm^3, apply the appropriate buckling terms - in general, leaking out in the thermal and streaming in in the fast groups - and calculate the spectrum by a source iteration process. The resulting k_{eff} is rather meaningless in this case; it gives, however, an estimate of the contribution of fission neutrons to the total fast source which should be negligible for properly chosen bucklings. The convergence of the source iteration is rapid enough, so that a good guess of k_{eff} is unnecessary which, anyway, would be difficult to obtain. Values in the order of 10^{-2} for k_{eff} are experienced.

Owing to the necessary addition of a fissile isotope it is not advisable to use the macroscopic cross sections so obtained for subsequent calculations, but to repeat the case without the fissile nuclide and to employ the fluxes previously evaluated (see input specification option 5, column 48 of Card No. 4).

A second possibility for calculating reflector cross sections is described in the next paragraph. This method, however, assumes that 18 group fluxes, e.g. from a ZOOM run [2] with provisional reflector data, are already known.

2.3 Evaluation of a 43 Group from an 18 Group Spectrum

The one-dimensional criticality programme ZOOM [2] solves the diffusion equations in up to 18 energy groups and can therefore generate a neutron spectrum which is quite accurate although the group cross sections used may not be averaged over the appropriate spectrum. For further application, especially for two-dimensional programmes, it is desirable to condense these 18 groups to, let us say, 6 groups. Two ways are feasible; one is to condense the basic 43 group data of MUPO in a first step to 18 groups by a flat flux assumption, and the other is to reconstruct a 43 group spectrum by interpolation from 18 groups.

Either the 18 or the 43 group cross sections can subsequently be condensed to any lower number of groups.

Because of its higher accuracy and greater flexibility the latter method was chosen. Reconstructing the 43 group spectrum also offers the opportunity of improving the original set of 18 group data when one condenses to the same 18 group structure. Furthermore, the ZOOM run can be repeated and a better flux spectrum obtained. Such a method is especially valuable when calculating reflector data. In this case the flux varies slowly with energy and therefore the interpolation procedure gives more accurate results.

The calculating method followed is described in the following. The flux spectrum is divided into three parts, the thermal, the epithermal and the fast. At thermal energies a second order polynomial is used for fitting:-

$$\phi_n(E) = A_n + B_n E + C_n E^2 \qquad 1 \leq n \leq 8 \qquad (6)$$

with

$$\psi_{n-1} = \int_{E_{n-2}}^{E_{n-1}} \phi_n(E)\, dE$$

$$\psi_n = \int_{E_{n-1}}^{E_n} \phi_n(E)\, dE \qquad 1 \leq n \leq 17 \qquad (7)$$

$$\psi_{n+1} = \int_{E_n}^{E_{n+1}} \phi_n(E)\, dE$$

where ψ_n are the group fluxes (between energies E_n and E_{n+1}) in 18 groups. The coefficients A_n, B_n, C_n of equation (6) are determined by solving the three equations (7). Then the fine group fluxes are evaluated:-

$$\Phi_m = \int_{E_m}^{E_{m+1}} \phi_n(E)\, dE \qquad E_{n-1} \leq E_m \leq E_{m+1} \leq E_n \qquad (8)$$

By this means it is ensured that the sum of the fine group fluxes within one broad group is equal to the broad group flux. The flat flux assumption is substituted by employing the fluxes of the next lower and higher broad groups.

The same is valid for the epithermal region. Here the fine group fluxes are obtained using equation (9) instead of (6):-

$$\phi_n = \phi_{on} \left(\frac{E_{on}}{E} \right)^{\nu_n} \qquad 9 \leqslant n \leqslant 17 \qquad (9)$$

Only two essential parameters are available for the three equations (7); first ν_n is evaluated from group fluxes (n-1) and (n+1) by a least squares fit and then ψ_n is used for the normalisation. The change-over from thermal to epithermal equation occurs between the eighth and ninth broad groups and should happen at an energy fairly close to the Maxwellian peak.

For the highest energy groups, however, equation (9) does not give satisfactory results and:

$$\phi_n(E) = \phi_{o_{18}} \left(1 - \frac{E}{E_o} \right)^{\nu_{18}} \qquad n = 18 \qquad (10)$$

is applied instead. E_o is the highest neutron energy, commonly E_o = 10 MeV. To simplify programming it is assumed that the last broad group is made up from three fine groups, and for these only equation (10) holds. The two parameters $\phi_{o_{18}}$ and ν_{18} are calculated by using the highest broad group flux ψ_{18} and the highest fine group flux ϕ_{40} obtained by the epithermal equation (9).

Experience has shown that the accuracy of this spectrum evaluation is better than 3% for the single fine group flux when applied to a Dragon reactor core spectrum. Of course, reaction rates averaged over several groups are much more accurate, especially for reflector regions.

2.4 The Calculation of Condensed Group Cross Sections

As already mentioned, MUPO was mainly written to provide few group cross sections needed as input for a number of other programmes. Therefore several options are included in the programme to produce cross sections on cards directly suitable for the one-dimensional criticality programme ZOOM [2], the two-dimensional criticality codes ANGIE [3] and CRAM [9]*, and finally the one-dimensional burn-up programme FEVER [6].

Having obtained the 43 group neutron spectrum by one of the six options the programme proceeds to calculate macroscopic condensed cross sections in much the same way as STEWPOT does; the transport mean free path, the absorption and scattering matrix, and the fission matrix (see [1], Section 2.3). The diagonal terms of the absorption and scattering matrix are the total cross sections, the remaining terms give the up-scattering (lower triangle) and the down-scattering (upper triangle). The elements of the fission matrix are the neutron production cross sections from group j to i ($\nu y_i \Sigma_{fj}$). All these cross sections are divided

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*This addition is due to Mr. J. Blomstrand

by the diffusion coefficient (one third of the transport mean free path) corresponding to that row.

The macroscopic cross sections are followed by the microscopic, total neutron production, transport and absorption cross sections for each isotope mentioned in the input data. When a FEVER Library is produced the same cross sections are punched on cards plus the scattering out cross sections for graphite and the ν-values for the fissionable isotopes.

ANGIE asks for data in the sequence capture, fission, transport, scattering out and the probability for up-scatter into the next higher and down-scatter into the next and next but one lower groups. Additionally, one ν-value for the whole core and the relative fission spectrum have to be supplied. In order to allow for a mixture of fissionable nuclides and to account for the fact that no capture cross sections are used by MUPO, it was necessary to modify the meaning of the cross section blocks (dashed values correspond to the original meaning in ANGIE):-

$$\Sigma'_{cj} = \Sigma_{aj} - 0.1\,\nu\Sigma_{fj}$$

$$\Sigma'_{fj} = 0.1\nu\Sigma_{fj}$$

$$\nu' = 1.0$$

$$y'_j = 10\,y_j$$

The division of the neutron production cross section by ten was necessary to avoid negative cross sections. No change in the criticality calculation of ANGIE will occur, likewise not in the power density as only relative densities are listed. A small error in the power density happens when two fissile nuclides are present in the core in different concentration ratios; but this case would have been treated even more falsely by the original ANGIE arrangement. All other cross sections have the original significance. For ZOOM the same method is observed.

No such modifications are necessary for the CRAM input preparation. The relative fission spectrum is given first followed by the transport, total and neutron production cross sections. The transfer cross sections are written row-wise, the diagonal terms put to zero.

All cross sections calculated in these options are printed and punched on cards.

2.5 The MUPO Library Tape

As already mentioned the programme is able to generate its own library tape by reading the necessary nuclear data from cards. After having read these cards it will produce a complete listing of all the data as a check and print the library summary before starting with the actual calculation.

The tape is written in roughly the following sequence:

tape identification number, title, total number of absorbers, of resonance tables, of scattering matrices,

energy-boundaries, fission spectrum

names of all isotopes

the cross sections for every isotope in the sequence σ_{tr}, σ_a, $\nu\sigma_f$, σ_f, in 43 groups

title for resonance table

names of all isotopes for which resonance tables are provided

the resonance tables themselves

title for scattering kernels

names of all scattering kernels

the kernels themselves.

All data appear with lowest energy first. They are terminated by an "end of file" mark.

A few words are necessary to explain the significance of the resonance tables. They are two parametric tables with not more than 80 entries. Each entry contains these two parameters and the equivalent set of 23 resonance absorption cross sections, starting with group 21 up to 43. This limitation is justified considering the fact that the lowest lying resonance normally treated in these calculations is at 6.7 eV (U-238).

In the present version the fuel temperature T_F and the σ_p-value are chosen as the two parameters. The absorption cross sections without 1/v part are calculated by:

$$\sigma_a(E_1, E_2) = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{\sigma_a(E)}{1 + \frac{\sigma_a(E) + \sigma_s(E)}{\sigma_p}} \cdot \frac{dE}{E}$$

using Blake's method and programme [8].

In order to cover the whole range of possible σ_p-values, from about 100 barns, for very lumped, up to 10^6 barns, for very diluted, resonance absorbers, it was necessary to choose carefully the step $\Delta\sigma_p$ between two successive σ_p-values for limiting the interpolation error. Assume the dependence of the resonance integral I from the σ_p-value is given by:

$$I = f(\sigma_p)$$

then it follows approximately that for

$$\Delta\sigma_p \approx \sqrt{\frac{8\,\varepsilon\, f(\sigma_p)}{\left| f''(\sigma_p) \right|}}$$

the relative error for linear interpolation is smaller than ε.

It was found, that 20 σ_p-values are sufficient to cover the whole range of interest and to guarantee an accuracy better than 0.5%. The σ_p-values chosen are listed below.

σ_p-Values (barns) used for Resonance Table

100	4450
160	6400
250	9200
390	13600
580	21000
840	34000
1190	60000
1660	120000
2330	300000
3200	1000000

By the same method four temperatures, 300, 750, 1300, 2000°K were selected giving in total 80 entries.

After having read from the library tape the resonance table for an isotope used in the calculation the programme scans the table for the four nearest entries (combination of the two parameters) and calculates the resonance absorption cross sections for the two specified parameters by linear interpolation.

The scattering matrices are to be written column-wise, the most thermal group first. The diagonal term is the total scattering out cross section (positive), whereas the transfer cross sections are given negative, so that the sum of each column is zero. In order to save time during read-write tape instructions and to gain core-storage, zeros can be omitted. Instead, the remaining numbers of each column are headed by a significant number in the form:

$$p + 0.01\ q + 0.0001 \qquad \begin{matrix} 0 \leq p \leq 41 \\ 1 \leq q \leq 42 \end{matrix}$$

p is the number of zeros to be inserted in front of the scattering cross sections provided and (42 - q) gives the number of zeros necessary to complete this column.

A detailed specification of the input to produce a library tape is given in the section "Input Preparation for Generating the Library Tape."

3. MISCELLANEOUS INFORMATION FOR THE USER OF THE PROGRAMME

3.1 Preparation of Input Data

The following cards have to be supplied directly after the "data" card, when running a problem.

Card No. 1:

Columns 1-36	any alphanumeric title, to identify data deck (will not be printed out).
Column 40	= 0: no print out of nuclear data on magnetic tape other than the summary.
	= 1: complete listing of these data.
Columns 41-44 (Int.)	ID number of LIBRARY Tape; when blank, ID number is not checked.
Card No. 2:	partition vector
Columns 1-3	total number of groups ≤ 18.
Columns 4-6	upper group number of first condensed group.
Columns 7-9	upper group number of second condensed group and so on.

For each case to be run the following set of cards has to be specified:-

Card No. 3:	blank
Card No. 4:	
Columns 2-24	title, case identification.
Columns 25-30 (Int.)	moderator temperature (^{o}K) for scattering kernel.
Columns 31-36 (Int.)	fuel temperature (^{o}K) for resonance absorption (first parameter in resonance tables).
Columns 37-42 (Int.)	total number of materials ≤ 110.
Column 48 (Int.)	mode of flux calculation (see section 2.1)

This integer specified how the programme obtains the 43 group fluxes necessary for the condensation of the scattering matrix and the microscopic and macroscopic data:

= 1: programme calculates the critical spectrum of an infinite homogeneous reactor by changing

the concentration of an absorber with arbitrary spectrum, when columns 61-72 are not blank or zero. (Case 1).

= 1: programme iterates on buckling when columns 61-72 are blank. (Case 3).

= 2: programme calculates the critical spectrum of a finite homogeneous reactor with an energy-dependent reflector saving or leakage rate by a source iteration process, see Columns 61-72. (Case 2).

= 3: programme reads a set of 18 group fluxes and evaluates 43 group fluxes.

= 4: programme reads a set of 43 group fluxes.

= 5: programme uses the 43 group fluxes of the previous case for the subsequent condensation of cross sections.

If options 4 or 5 are used, no flux guess (Columns 61-72) is necessary as this number is meaningless.

Columns 49-54 (Int.) — total number of materials for which disadvantage factor shall be applied.

Column 60 — mode of print out:

= 0: no calculation of ANGIE and ZOOM input data.

= 1: print out and cards for ANGIE input data.

= 2: print out and cards for ZOOM input data.

= 3: print out and cards for ANGIE and ZOOM input.

= 4: the 43 group fluxes are punched on cards in the same format as they are accepted by the programme.

= 5: print out and cards for FEVER Library.

= 6: print out and cards for CRAM input data.

Columns 61-72 (Float) — guess for flux calculation.

Case 1 — for spectrum calculation with absorber: it is the estimated concentration (10^{24} atoms/cm^3) of the absorber necessary to obtain a critical reactor.

If guess negative: the programme expects 43 absorption cross sections

to be read in.

If guess positive: the programme calculates 43 absorption cross sections for a 1/v - law with a 2200 m/sec cross section of one barn.

Case 2 for spectrum calculation by source iteration: the guess value is the estimated k_{eff} of the critical reactor.

If guess negative: the programme expects energy-dependent leakage in 43 groups and starts with the absolute amount of the guess.

If guess = 0: programme assumes no leakage (infinite homogeneous reactor) and starts with $k_{\infty} = 1.1$.

If guess positive: programme assumes no leakage and starts with the guess.

Case 3 for spectrum calculation with buckling iteration: leave Columns 61-72 blank.

The programme iterates on the buckling - assumed to be the same in all groups - until criticality is achieved. It starts with a buckling of 10^{-4} cm^{-2}.

Card No. 5:

Columns 1-24		material specification of first material.
Columns 25-48		material specification of second material.
Columns 49-72		material specification of third material.
Specification for every material	I4	material number.
	F7.0	σ_p-value for resonance materials (barns) (second parameter in the resonance tables)
	E13.5	concentration (10^{24} atoms/cm^3). (Can be zero).

The next material has to be specified in Columns 25-48 in the same sequence, the next but one in 49-72, if more materials a second and third, etc., "Card 5" have to be used. The various isotopes have not necessarily to be given in the order of increasing material number.

Card No. 6: the following group of cards defines the disadvantage factors if any.

One blank card followed by 4 cards whereby the first value gives the material number proper followed by 43 disadvantage-factors. (12 per card).

This block of 5 cards has to be repeated for as many materials as specified on Card No. 4, Column 54.

Card No. 7: the next group of cards is only necessary if either (a) energy-dependent absorption, respectively leakage will be used or (b) fluxes as input data are provided. Thermal data have to be given first.

(a) energy-dependent absorption or leakage:

one blank card followed by 8 cards which specify the 43 group absorption cross sections (barns), respectively bucklings (cm^{-2}) in 43 groups (6 per card).

(b) fluxes as input data: 43 or 18 fluxes (6 per card). Add a second Card No. 2 with the partition vector of the 18 group fluxes when appropriate.

A next case has to be started by Card No. 3.

3.2 Operating Instructions

The library tape should always be "file protected". It is written in high density. There are no special operating instructions other than the normal 7090 Fortran-monitor instructions. The calculation time is very much dependent on the number of cases; one single case will take about one minute, but running-time of as little as 10 seconds per case were experienced when many cases were run.

3.3 Tape Assignment

As there is no rule generally accepted by computing centres which function the various input-output devices hold, provision is made that the tape assignment can easily be changed by altering the first four instructions of the symbolic deck. The table below gives the assignment used in the present version.

TABLE 1: Tape Assignment

Function	Integer Used	Logical Tape Unit*	Corresponding Channel	
			CEGB*	Risley*
Input	J2	2	A2	A2
Printed Output	J3	3	A3	A3
Punched Output	J8	8	B4	B4
Mupo Library	J9	9	A5	C1

*present version

3.4 Errors in Input Deck

The following section should assist the programmer in finding errors caused by a faulty input deck. Input data are printed immediately after reading in the case of Card No. 4 and Card No. 7. The content of Card No. 5 is printed after all 43 group cross sections and the appropriate resonance tables have been read from tape and the disadvantage factors of Card No. 6 have been applied.

When the user has specified a material number which is not in the Library, he will be notified and the material number printed. In case something is wrong with the disadvantage factors, either too many or too few, the programme reads subsequent cards, if any, or calls EXIT, or in the latter case reads the remaining disadvantage factors as something else. In both cases this error should be detected fairly easily by scrutinising the available print-out. When a block of disadvantage factors is designated to a material which is not listed on Card No. 5 a print-out will occur giving the false material number. Having completed this part of the programme, the name, concentration and σ_p-value of all isotopes used and their cross sections will be printed. Following this the tape is scanned for the scattering kernel; failure is indicated by "no scattering matrix available". As there is no possibility of the user's interfering with the tape reading by a faulty input deck, termination of a job by statements like "End of File" or "Redundance encountered" most certainly indicates that the tape got spoilt.

Prior to the spectrum calculations one line will be printed; "the critical spectrum ...." It may happen that no convergency in the spectrum calculation can be achieved when the isotope concentration is not the one of a thermal or epithermal graphite moderated reactor, e.g. no thermal fission takes place or the carbon concentration is too low.

Experience has shown that the source iteration process can lead to negative fluxes when too high negative bucklings are used, simply because the leaking in of neutrons is higher than the total absorption in that group.

When writing a new library tape errors can normally be found easily by attempting to obtain a complete listing. In this case only one blank card with a "1" in column 40 has to be provided after the programme itself and the "data" card.

3.5 Input Preparation for Generating the Library Tape

As already mentioned the programme generates its own library tape by reading the cross sections from cards. In the following a specification is given how to prepare the cards. For additional information see the section "The MUPO Library Tape".

Card No. 1

Columns 2-36	any alphanumeric title
Columns 37-40 (Int.)	number of absorbers (NI): $2 \leq NI \leq 110$
Columns 41-44 (Int.)	number of resonance materials (NJ): $1 \leq NJ \leq 5$

Columns 45-48 (Int.)	number of scattering matrices (NK): $1 \leq NK \leq 27$ to be read
Columns 49-52 (Int.)	identification number of tape (ID): $1 \leq ID$

For the following, cross sections and data are to be listed in order of increasing energy.

Card No. 2	44 energy boundaries (in eV) (6 per card)
Card No. 3	9 numbers giving the relative fission-spectrum, sum is equal to 1.0 (6 per card)

The following cards Nos. 4-7 or 10 have to be supplied as often as advertised in Card No. 1 Columns 41-44.

Card No. 4

Columns 2-24	name of isotope (alphanumeric)
Columns 25-27 (Int.)	identification number of isotope. It has to be chosen in increasing order so that the highest identification number is identical with the total number of absorbers.
Columns 28-36 (Float)	ν-value (for identification of fissionable materials).
Card No. 5	43 transport cross sections (6 per card)
Card No. 6	43 absorption cross sections (6 per card)
Card No. 7	blank

In the case of fissionable isotopes the following cards (Nos. 8-10) have to be provided as well.

Card No. 8	43 neutron production cross sections ($\nu \cdot \sigma_f$). (6 per card)
Card No. 9	43 fission cross sections. (6 per card).
Card No. 10	blank

Card No. 11

Columns 2-36	alphanumeric title for resonance tables
Columns 37-48 (Float)	epithermal scattering cross section of moderator (used to evaluate the homogeneous σ_p-value)
Card No. 12	blank

The following cards Nos. 13-16 have to be supplied as often as advertised in Card No. 1 Columns 45-48.

Card No. 13

Columns 2-36	alphanumeric title for resonance absorber
Columns 37-40 (Int.)	material identification number
Columns 41-44 (Int.)	number of entries in resonance table (≤ 80)
Columns 49-60 (Float)	potential scattering cross section of absorber

Cards No. 14 and 15 have to be repeated for every entry.

Card No. 14

Columns 1-15	any alphanumeric title (not used)
Columns 16-21 (F.6.1)	first parameter for resonance table (Temperature ^{o}K)
Columns 22-32 (F.11.1)	second parameter for resonance table (σ_p-value) 5 resonance absorption cross sections (F.8.4).
Card No. 15	the remaining 18 resonance absorption cross sections (9 per card in format F.8.4)

The entries are to be given in such a sequence that the second parameter covers the whole range in increasing order before the first parameter is changed to a higher value.

Card No. 16	blank

Card No. 17

Columns 2-36	alphanumeric title for scattering matrices

Cards No. 18-20 have to be supplied as often as indicated in Card No. 1 Columns 45-48.

Card No. 18	blank

Card No. 19

Columns 2-36	alphanumeric title for scattering matrix
Columns 37-48 (Float)	temperature of kernel in ^{o}K
Columns 49-54 (Int.)	total number of scattering cross sections and significant numbers to follow (≤ 700)
Card No. 20	scattering cross sections and significant numbers (7 per card in the format F.10.6)

The different scattering kernels have to be given with increasing temperature.

Integers (Int.) have to be written at the utmost right of the specified field, (Float) means the number can be given either as a floating or fixed point decimal. The same is valid in the case where "6 per card" is stated, which means that a field of 12 columns is reserved for every number. It is obvious that by using the floating point form the exponents has to be written to the utmost right of the field. When the format is specified as, e.g. F.8.4 the number has to be supplied with fixed decimal point in a field of 8 columns. When the last four columns in the above example are occupied by the decimal part, and only then, the decimal point can be omitted.

These data will be read on logical tape unit 9 in the present version of the programme; however, this tape assignment can easily be changed by altering one of the first instructions in the symbolic deck which specify the tape used. For calculations at C.E.G.B. London, logical tape unit 9 is equivalent to channel A5 and at Risley it is channel C1.

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