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MINX:

A Multigroup Interpretation of Nuclear X-Sections from ENDF/B

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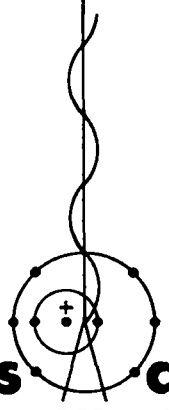

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ABSTRACT

MINX calculates fine-group averaged infinitely dilute cross sections, self-shielding factors, and group-to-group transfer matrices from ENDF/B-IV data. Its primary purpose is to generate pseudo-composition independent multigroup libraries in the standard CCCC-III interface formats for use in the design and analysis of nuclear systems. MINX incorporates and improves upon the resonance capabilities of existing codes such as ETOX and ENDRUN and the high-Legendre-order transfer matrices of ETOG and SUPERTOG. Group structure, Legendre order, weight function, temperature, dilutions, and processing tolerances are all under user control. Paging and variable dimensioning allow very large problems to be run. Both CDC and IBM versions of MINX are available.

I. INTRODUCTION

The ENDF/B file[1] is the United States reference nuclear data base containing evaluations of cross sections, derived from experimental measurements and nuclear model calculations, in a form suitable for automated retrieval and processing. The MINX[2,3] code is a new, designer-oriented, multigroup cross-section processing code which reads the ENDF/B file and produces multigroup and point-wise data for a wide variety of problems in nuclear systems design and analysis. MINX is jointly sponsored by the Division of Reactor Research and Development and by the Division of Military Applications of the United States Energy Research and Development Administration. The code and the multigroup data sets derived therefrom are intended to satisfy the nuclear design standards[4] currently being implemented under auspices of the American National Standards Institute. The program is

being developed in successive versions; the neutron capabilities of Version I is described herein.

Version I of MINX is intended to incorporate and improve upon the resonance capabilities of existing codes such as ETOX[5] and ENDRUN[6] and the high-order group-to-group transfer matrices of SUPERTOG[7] and ETOG.[8] MINX is the first link of a two-step process; it generates a fine multigroup library with group-dependent resonance self-shielding factors from ENDF/B data. The SPHINX[9] code, the second step, interpolates to the correct composition-and temperature-dependent self-shielding factors, and space-energy collapses the resulting cross sections to the desired group structure. The breakup in this fashion[10] permits detailed physics mechanisms to be treated with rigor by an infrequently run MINX program, and survey design calculations to be performed rapidly by an often-used SPHINX program. The MINX and SPHINX programs are linked through standard interfaces.[11]

II. GENERAL FEATURES OF MINX

A. Temperature-Dependent Pointwise Library

MINX generates and uses a linearly interpolable, infinitely dilute, temperature-dependent pointwise cross-section library in ENDF/B format.[12,13] (Cross sections for the same nuclide at different temperatures have the same material number.) Self-shielding is treated in subsequent processing stages.* This feature permits efficient computation of group cross sections with accurate Doppler broadening[13-16] of single-level and multilevel cross sections. The multigroup constants generated therefrom are thus known to be compatible with the pointwise cross sections retrieved by continuous-energy Monte Carlo codes.[13,17] Those "background" cross sections artificially introduced by the evaluator in the single-level representation of multilevel interference effects are also naturally broadened and self-shielded within the framework of this formalism. In those cases where the resonance component is significantly reduced due either to self-shielding or Doppler broadening, the self-shielding of an oscillating positive and negative background may be significant.

B. Reference Frame for Differential Scattering Cross Section Employed in Transfer Matrix Calculation

Traditionally, angular distributions for two-body interactions have been provided in ENDF/B in the center-of-mass system, possibly because of the guidance

*The unresolved region is a special case for which Doppler broadening and self-shielding are considered simultaneously.

lent by results of model calculations performed in this system and because, traditionally, physicists tend to report data in this system. This approach is not necessarily the most desirable. Indeed, experimental measurements are performed in the laboratory system. For those situations in which laboratory angular distributions are provided directly (formats for this representation are permitted in ENDF/B-IV) or obtained through transformation from center-of-mass to lab, new and accurate algorithms[18] can be employed for the computation of group-to-group matrices. These calculations are based upon a semianalytic procedure which treats the rapidly fluctuating cross-section behavior analytically. These algorithms require only a minimum of numerical approximations and use recursive formulas well suited to performing the required integrations. A flexible energy integration mesh is employed so that localized resonance phenomena may be adequately represented. The approach does depend, however, on deriving a suitable Legendre series expansion of the angular distribution in the laboratory system. Where this becomes too time consuming (e.g., for light nuclei or near inelastic thresholds), an alternative numerical integration in the center-of-mass system is employed.

C. Bondarenko Representation

The Bondarenko[19] scheme of employing table sets to account for temperature and dilution effects was chosen for the MINX/SPHINX system because of its economy and wide acceptance by the community of reactor designers. It allows MINX to compute multigroup microscopic cross sections separately for each nuclide, the influence of the nuclear environment being reflected through input flux weighting spectra, through background cross sections and equivalences, and through temperature and other material parameters.

This method is based on the narrow resonance approximation. It is most appropriate for large systems containing some light elements, but various extensions are being explored.[20,21] The question of the adequacy of table interpolation as opposed to on-line computation for the flux for the system of interest has only begun[10] to be systematically addressed in terms of accuracy gained for a given computational time penalty.

D. Uncertainty Estimates

Recognized uncertainties in nuclear data have brought increasing attention to the determination of nuclear design uncertainties consequent to uncertainties in nuclear data. A component of this uncertainty is that introduced in processing the data. Hence the algorithms employed for constructing, interpolating, and

integrating cross sections in MINX are intended to provide user control of computational errors (provided one assumes that the data base and weighting function are known explicitly). The attempt to assign uncertainties due to multigroup processing procedures is still under active development, particularly with respect to combining uncertainties (which are clearly correlated) introduced and quantified at various stages of the processing. The goal of computing multigroup constants to within some given accuracy assignment has, in many cases, led to "over kill" and long processing times to achieve accuracies in some elements of the multigroup data which may not merit such attention for specific problems. The user control has, however, been extremely valuable in determining the sensitivity of multigroup constants to factors such as integration mesh, Legendre series expansion truncation, and for general debug analysis. Since the design of MINX was such that it was expected to be run very infrequently, the longer processing times were accepted in the spirit of achieving the goal of reducing the relative error in the processing to some known measure, well below existing uncertainties in nuclear data. As with most computer program developments, a tradeoff always exists between accuracy and speed.

E. Paging Techniques and Variable Dimensioning

The paging technique developed initially in the RESEND[22] code was incorporated in MINX for the reconstruction of pointwise cross sections from resonance parameters. It involves the manipulation of cross-section information one block at a time. This block size is variable and permits processing of large amounts of cross-section data without making huge storage demands on the computing hardware. The method is now employed throughout the MINX code including not only resonance reconstruction, but Doppler broadening, multigroup averaging, and computation of group-to-group matrices.

Efficient use of storage is essential in a large code like MINX. Variable dimensioning techniques are used which store data in a single long array (in blank common) using pointers to locate each quantity. No memory locations are left unused at the end of arrays as in fixed dimensioned codes and storage locations can be used for different variables at different times. With variable dimensioning and paging, very large problems can be run with MINX.

F. BCD Format Data Files

MINX uses the ENDF/B BCD formats[1] exclusively. The binary formats would provide more efficient input/output, but they do not permit partitioning of the very large cross-section vs energy tabulations required for data handling

of the pointwise library. Using BCD formats allows the data to be read in by "pages" of convenient size. In addition, the current ENDF/B-IV binary formats embed the lengths of tables to be read (such as interpolation, energy, cross section) in the records themselves, thus making it difficult to assign pointers for variable dimensioning without complex buffering schemes. In order to have a processing code which is truly variably dimensioned and efficient, it is suggested that the binary formats of ENDF/B be changed in the next version.

III. STRUCTURE AND STATUS OF MINX

MINX is coded in Standard FORTRAN-IV with data management, precision, and other features particularly adapted alternatively to CDC and IBM computers. MINX is currently operational on the CDC-7600 at Los Alamos Scientific Laboratory (LASL) and on the IBM 360/91 and 360/195 at Oak Ridge National Laboratory (ORNL). The code is modular in structure and its output conforms to guidelines developed by the Committee on Computer Code Coordination.[23] Many of the modules, such as SIGMA1[24] and RESEND[22] along with the ENDF/B utility modules, were provided by other laboratories participating in the ENDF/B system. Modular structure, among other advantages, opens possibilities of collaboration among developers of processing codes such as AMPX[25] and GALAXY.[26] Indeed, MINX and SPHINX have already been incorporated as part of the AMPX system.

The large-scale structure of MINX is illustrated in Fig. 1. Here the functional blocks illustrated correspond to CDC main and primary overlays. Each functional block typically contains secondary overlay levels and a number of modules.

All ENDF/B data for the material or materials being processed (labeled ENDF/B in the figure) are passed on BCD tapes from one functional block to another. In the main, RESEND adds to the data stream cross sections reconstructed from resolved resonance parameters; SIGMA1 Doppler broadens these; UNRESR adds self-shielded unresolved resonance contributions; TERROR computes the required multigroup constants; and FOURC writes the multigroup cross sections, f-factors, and matrices in CCCC-III format. ETOPL[13] formats cross sections for continuous energy Monte Carlo codes. It is not a part of the MINX package.

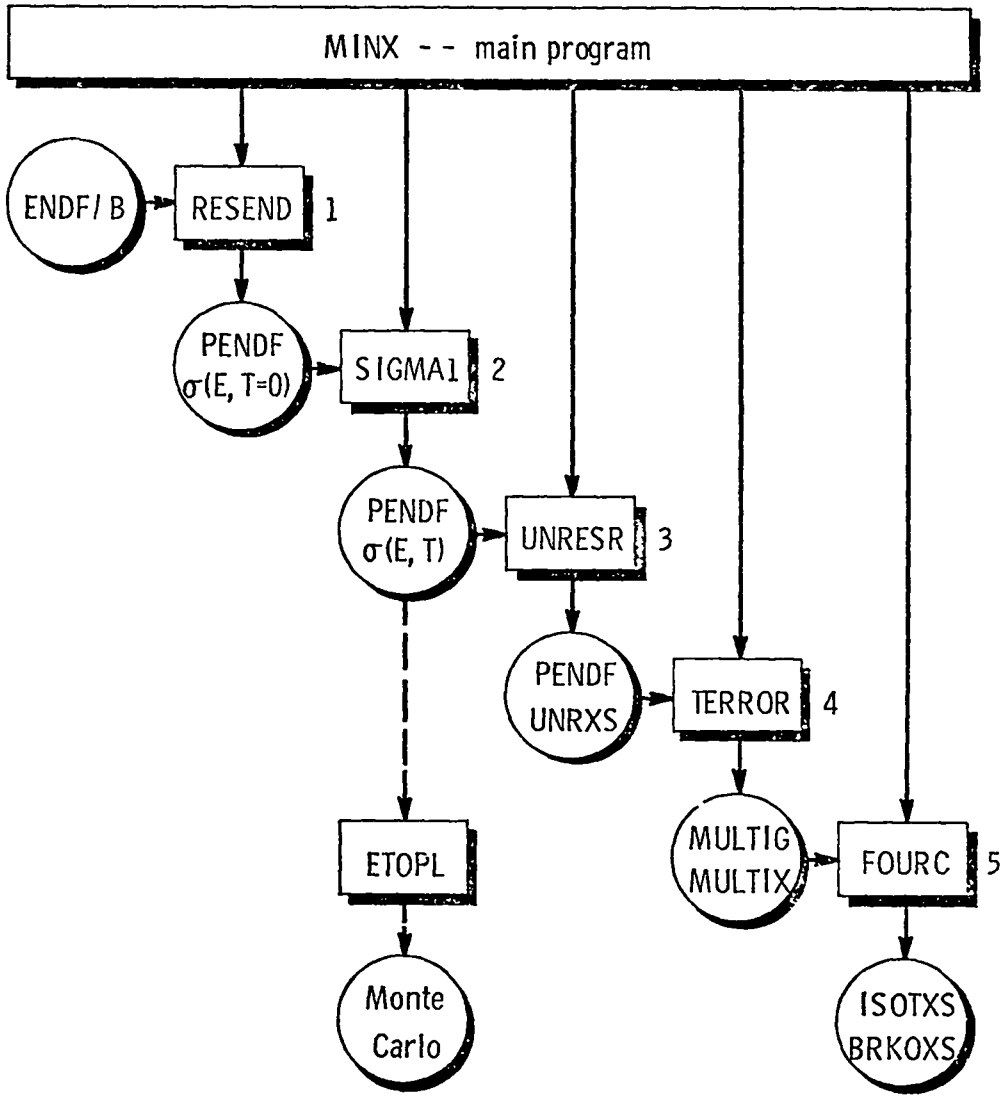

Fig. 1. Structure of MINX code illustrating functional blocks and data flow. ETOPL[13] is not a part of MINX.

IV. PROCESSING ALGORITHMS

A. Reconstruction of Infinitely Dilute Cross Sections (0 K) in the Resolved Energy Region from Resonance Parameters

Infinitely dilute, unbroadened point cross sections are obtained from resolved resonance parameters using a modified version of the RESEND[22] program. The code computes resonance contributions from File 2 in ENDF/B-IV, according to the formalisms specified in the ENDF Formats and Procedures Manual,[1] for total, elastic, fission,and capture cross sections. It then adds the background cross sections given in File 3. The ENDF/B parametric resonance representations are included in Appendix A for completeness and to establish notation.

The method used for reconstructing resonances is described in Appendix B. The resulting cross sections represent the true function to within some specified tolerance. The user must attempt to choose this accuracy criterion in a manner that insures the adequacy of the tabular files in the widest range of applications, yet results in the smallest number of points. Typically, tables with 10 000 to 50 000 points per reaction type are generated when major isotopes are reconstructed at 0 K with an accuracy of 0.1%.[27] (See Table I.) Such high accuracy files should be considered as a master data base which needs only to be generated rarely.

The modifications to RESEND involve principally input/output assignments, storage allocation, the construction of a new section for the potential scattering cross section (MT285), and a better procedure,[28] suggested by C. R. Lubitz, (Knolls Atomic Power Laboratory) and coded by P. F. Rose (Brookhaven National

TABLE I

DEPENDENCE OF TABLE SIZE ON ACCURACY SPECIFICATION

FOR TOTAL CROSS SECTION

% Accuracy	Number of Points in the Tabulation		
	U-238	U-233	Fe
0.5	69282	1881	4176
1.0	49943	1300	2944
2.0	35302	927	2004
5.0	22105	530	1263

Laboratory) to reformulate the calculation of multilevel Breit-Wigner elastic scattering interference terms (involving a summation of quadratic interference terms) so that the scattering resonance terms are summed before squaring.

After completion of this processing segment, a new ENDF/B tape (restriction to 5000 permissible energy points suppressed) is available in BCD format; File 2 data is bare (no resonance parameters), and File 3 contains the 0 K pointwise cross sections and unresolved-resonance cross sections at infinite dilution.

B. Exact Doppler Broadening of Tabulated Cross Sections

The SIGMA1 kernel broadening method[24,29] takes advantage of the tabulation of cross section vs energy (in ENDF/B format), with linear-linear interpolation between tabulated values. Under these conditions, the Doppler broadening equation is solved assuming only an isotropic Maxwell-Gas model describing the velocity distribution of the nuclei in the medium and nonrelativistic energies. The resulting algorithm is quite general, does not include any energy or temperature restrictions, and is equally applicable to neutron or charged particle cross sections.

The SIGMA1 module reads the output from the RESEND module. Any logarithmic or semilogarithmic representations are converted to linearly interpolable functions using the method described in Appendix C. The resulting linear-linear table is then Doppler broadened (see Appendix D), thinned (see Appendix E), and written onto the output "PENDF" file. This file is in ENDF/B BCD format except the 5000 point limit has been removed. Subsequent temperatures are then "bootstrapped" from the preceding temperature and written onto the PENDF file as additional "MATs" with the same material number but different temperatures. This procedure takes advantage of the smoothing effect of Doppler broadening to speed up the calculation. Paging is used throughout the calculation, so there is no limit on the number of energy points in the cross section being broadened.

The modifications made to SIGMA1 include the following: input parameters taken from COMMON, linearization routine added, selective material and temperature loops added, bootstrap and restart operation added, and broadening suppressed for high-threshold reactions.

C. Determination of Effective Temperature-Dependent Self-Shielded "Pointwise" Cross Sections in the Unresolved Energy Range

Since, by definition, in the unresolved energy range we do not know the cross-section value for any particular energy point, an expected value (symbolized by $\langle\ \rangle$) is taken over the distribution of resonance locations and widths.

The technique used follows (almost directly) that used in the ETOX[5] code (the technique was, in turn, adapted from the MC^2 code[30]). The effective cross section at energy E is then obtained by evaluation of Eq. (1). A special expression is formulated for the self-shielded total cross section due to its relationship to the transport cross section (see Appendix F).

$$\bar{\sigma}_x(E,T,s_o) = \frac{\left\langle \frac{\sigma_x(E,T)}{1 + \sigma_t(E,T)/\sigma_o} \right\rangle}{\left\langle \frac{1}{1 + \sigma_t(E,T)/\sigma_o} \right\rangle} \quad . \tag{1}$$

Unlike the resonance reconstruction and kernel broadening operations described in Sec. IV A and Sec. IV B, the composition-dependent parameter σ_o is introduced and Doppler broadening and self-shielding are done simultaneously in the UNRESR routine which computes effective (flux-averaged) cross sections for fission, capture, elastic scattering, and total. The primary modification to the ETOX algorithm is associated with the integration technique used to establish the mean values indicated in Eq. (1).[31] The selection of energy mesh points, at which the effective cross sections are calculated, has been modified to include the energy points given in the ENDF/B file or, if the energy-independent formalism was employed, points spaced at half-lethargy intervals. Effective cross sections at intermediate energy points are obtained by assuming that the cross sections vary linearly between these points. Finally, the storage of resonance parameters and background cross sections was changed for consistency with the RESEND module.

The explicit formulation for the UNRESR calculation is taken directly from the ETOX[5] program description and is included as Appendix F for completeness. The change in the quadrature scheme is due to the fact that the earlier scheme used in ETOX and MC^2 generally overestimates[31] both the capture cross section of fertile isotopes (~0.3 to ~0.5%) and the fission cross section of fissile isotopes (~1.5 to 2.0%), but underestimates its capture as a consequence of overweighting the points with large partial widths. Thus, the evaluation of the fluctuation integrals

$$\int_0^\infty P_\mu(x)dx \int_0^\infty P_\nu(y)f(x,y)dy = \sum_{j=1}^{N}\sum_{k=1}^{M} A_j A_k f(x_j,y_k) \quad , \tag{2}$$

is now carried out with the quadrature set[31] of Table II. The x's and y's represent the ratio of elastic and fission widths relative to the mean values at a particular energy of interest.

TABLE II

UNRESOLVED INTEGRATION QUADRATURE

Index (i)	Ordinates (X_i) Degrees of Freedom, (μ)			
	1	2	3	4
1	3.00135 - 3	1.32192 - 2	1.00045 - 3	1.32192 - 2
2	7.85929 - 2	7.23496 - 2	2.61976 - 2	7.23496 - 2
3	4.32824 - 1	1.90895 - 1	1.44275 - 1	1.90895 - 1
4	1.33453	3.95288 - 1	4.44842 - 1	3.95288 - 1
5	3.04818	7.40834 - 1	1.01606	7.40834 - 1
6	5.82632	1.34983	1.94211	1.34983
7	9.94526	2.52980	3.31509	2.52980
8	1.57821 + 1	5.23849	5.26071	5.23949
9	2.39968 + 1	1.38218 + 1	7.99894	1.38218 + 1
10	3.62162 + 1	7.56475 + 1	1.20721 + 1	7.56475 + 1

Index (i)	Weights (A_i) Degrees of Freedom (μ)			
	1	2	3	4
1	1.11204 - 1	3.37734 - 2	3.33762 - 4	1.76238 - 3
2	2.35468 - 1	7.93322 - 2	1.85061 - 2	2.15177 - 2
3	2.84410 - 1	1.28359 - 1	1.23099 - 1	8.09798 - 2
4	2.24191 - 1	1.76526 - 1	2.99189 - 1	1.87980 - 1
5	1.09677 - 1	2.13470 - 1	3.34315 - 1	3.01563 - 1
6	3.04938 - 2	2.11550 - 1	1.77666 - 1	2.96161 - 1
7	4.29309 - 3	1.33652 - 1	4.26959 - 2	1.07756 - 1
8	2.58270 - 4	2.26306 - 2	4.07606 - 3	2.51719 - 3
9	4.90320 - 6	1.63136 - 5	1.17661 - 4	8.93604 - 10
10	1.40792 - 8	2.74538 - 31	5.09895 - 7	1.16454 - 61

D. Calculation of Group-Averaged Cross Sections and Self-Shielding Factors

Assuming a weighting function of the form

$$\phi^i(E,T,\sigma_o) = \frac{C(E)}{\sigma_t^i(E,T) + \sigma_o} \quad , \tag{3}$$

where

$\phi^i(E,T,\sigma_o)$: represents the Bondarenko model for the energy dependent flux to be used with this isotope,

$C(E)$: represents the broad energy behavior of the spectrum (e.g., 1/E, fission spectrum),

$\sigma_t^i(E,T)$: is the energy-dependent total cross section at temperature T for the isotope of interest, and

σ_o : macroscopic total cross section per atom of the isotope of interest (spatial and lattice effects are subsequently deduced by incorporation of equivalence principles through σ_o parameter).

The group-averaged cross section of type x, for energy group g, of isotope i, at temperature T, in a mixture of dilution σ_o is

$$\bar{\sigma}_{xg}^i(\sigma_o,T) = \frac{\int_g \phi^i(E,T,\sigma_o)\sigma_x^i(E,T)dE}{\int_g \phi^i(E,T,\sigma_o)dE} \quad . \tag{4}$$

Self-shielding or "f-factors" are then defined by

$$f_{xg}^i(\sigma_o,T) = \frac{\bar{\sigma}_{x,g}^i(\sigma_o,T)}{\bar{\sigma}_{x,g}^i(\infty,0)} \quad . \tag{5}$$

A special "total" cross section is calculated as

$$\bar{\sigma}_{t,g}^i(\sigma_o,T) = \frac{\int_g \frac{\sigma_t^i(E,T)C(E)dE}{[\sigma_t^i(E,T)+\sigma_o]^2}}{\int_g \frac{C(E)dE}{[\sigma_t^i(E,T)+\sigma_o]^2}} \quad , \tag{6}$$

reflecting the current weighting appropriate to its role in the transport equation (a slightly different form is used in the unresolved region). The justification for this flux assumption is discussed in Appendix G.

Group cross sections are obtained by performing an integral of the type in Eq. (4) in all energy ranges. Outside the unresolved range, the point cross sections are retrieved by linear interpolation from the PENDF file described in Sec. IV B. Inside the unresolved range, the average cross sections are retrieved by linear interpolation from a file written by the UNRESR module discussed in Sec. IV C. The integral over energy for each group is divided into a set of panels defined by the union of the grid points for each of the functions appearing in the integrand of Eq. (4). Since the energies at which the cross sections are tabulated were chosen such as to represent the "true" behavior to a specified accuracy, it is highly unlikely that any significant structure is missed. The integration scheme actually employed in MINX is adaptive and based on Simpson's method.[32] Such a scheme was chosen in the spirit of quantifying the integration accuracy (for arbitrary behavior of an integrand) by convergence based upon adaptive iteration techniques. It is also common to integration performed elsewhere in MINX (e.g., transfer matrices). However, it should be noted that such schemes are generally quite time consuming and further work is currently underway to provide accuracy assurance with simpler, faster schemes. Infinitely dilute cross sections are generated for all reactions appearing on the ENDF/B tape (or specified reactions, if desired) as well as the average number of neutrons per fission ($\bar{\nu}$), the average scattering cosine ($\bar{\mu}$), and the average logarithmic energy decrement ($\bar{\xi}$). The last three quantities are computed at 0 K as follows (temperature variable suppressed)

$$\bar{\nu}_g^i = \frac{\int_g \bar{\nu}^i(E)\sigma_f^i(E)C(E)dE}{\int_g \sigma_f^i(E)C(E)dE} , \tag{7}$$

$$\bar{\mu}_g^i = \frac{\int_g \bar{\mu}^i(E)\sigma_e^i(E)C(E)dE}{\int_g \sigma_e^i(E)C(E)dE} , \quad \text{and} \tag{8}$$

$$\bar{\xi}^i_g = \frac{\int_g \bar{\xi}^i(E)\sigma_e(E)C(E)dE}{\int_g \sigma_e(E)C(E)dE} \quad . \tag{9}$$

Self-shielding factors are computed for the total, elastic, capture, fission, and transport cross sections. The self-shielding factor for the elastic scattering cross section is applied to the infinitely dilute transfer matrices (discussed in the next section). The transport cross section is calculated using

$$\sigma^i_{tr,g}(\sigma_o,T) = \sigma^i_{t1g}(\sigma_o,T) - \bar{\mu}^i_g \sigma^i_{e,g}(\sigma_o,T) \quad , \tag{10}$$

where σ^i_{t1g} is the current weighted total cross section defined through Eq. (6).

E. Calculation of Multigroup Transfer Matrices for Two-Body Interactions Using the Laboratory System

Most previous methods for the calculation of multigroup transfer matrices for elastic and discrete inelastic scattering involve integrals of the form

$$\int_{\omega_{g-1}}^{\omega_g} I(u)P_j(\omega_L)P_k(\omega_c)d\omega_c \quad , \tag{11}$$

with u representing the incident neutron lethargy, ω_L and ω_c being the cosines of the scattering angles in the laboratory and center-of-mass systems respectively, I(u) representing collision density type terms, and the P's standing for Legendre polynomials. Since the lethargy is related to ω_c via a logarithm, and ω_L is related to ω_c via a square root, the integral rapidly becomes quite involved since the resulting expressions include integrals of $P_j(\omega_L)$ and $P_k(\omega_c)$ evaluated over finite limits.

If the scattering angular distributions are expanded in the laboratory system rather than the center-of-mass, and the sink group integration performed in the laboratory cosine variable, then the algebra may be considerably simplified and the computing complexity reduced. This scheme is developed in detail in Ref. 18.

Such a formulation leads to expressions for the group-to-group cross sections of the form

$$\sigma^{j}_{g'\to g} = \frac{\int_{E_{g'}}^{E_{g'-1}} N_j(E')\sigma(E') \sum_{k=0}^{K} \frac{2k+1}{2} f_k(E') \int_{\omega_{g-1}}^{\omega_g} P_j(\omega)P_k(\omega)d\omega\, dE'}{\int_{E_{g'}}^{E_{g'-1}} N_j(E')dE'} , \tag{12}$$

where

$\sigma^{j}_{g'\to g}$ = j^{th} component of the group-to-group cross section for neutron scattering from group g' to group g,

$E_{g'}, E_{g'-1}$ = lower and upper energy boundaries for group g' ,

$N_j(E')$ = j^{th} component of the weighting function at energy E' ,

$\sigma(E')$ = cross section for the two-body reaction at energy E' ,

$\sum_{k=0}^{K}$ = summation of K + 1 terms describing the scattering angular distributions in the laboratory system ,

$f_k(E')$ = k^{th} expansion coefficient of the laboratory angular distribution ,

$P_j(\omega), P_k(\omega)$ = Legendre polynomials of argument ω, order j and k , respectively , and

ω_g, ω_{g-1} = laboratory cosines fixed by the scattering process for particular source energy E' and sink group boundaries E_g and E_{g-1}, respectively.

It is noteworthy that the entire inner integral, which contains rapidly fluctuating terms, is analytically integrable. Furthermore, its integrand is

symmetric in j and k, and the Legendre polynomials are easily amenable to recursive analysis. If

$$Y_{jk} = \int_a^b P_j(\omega) P_k(\omega)\, d\omega$$

$$Y_{-1,k} = Y_{j,-1} = 0 \quad , \tag{13}$$

then

$$Y_{j,k+1} = \frac{2k+1}{k+1}\left(\frac{j+1}{2j+1}\right) Y_{j+1,k} + \frac{2k+1}{k+1}\left(\frac{j}{2j+1}\right) Y_{j-1,k} - \frac{k}{k+1} Y_{j,k-1} \quad . \tag{14}$$

The integration limits a and b are determined through the kinematics of the scattering process[18] and the relation to the multigroup energy boundaries.

Thus, the determination of multigroup transfer matrices is reduced to the numerical evaluation of a single integral. This is performed with an adaptive Simpson[32] method which uses a flexible energy mesh so that localized resonance phenomena may be adequately represented. The integration technique is iterative and converges to within a specified tolerance, utilizing an appropriate number of points depending upon the variation of the integrand. Computationally, it is important that the summation over k be inside the outer integration.

In the development leading to Eq. (12), the scattering cross sections are assumed to be independent of the direction of the incoming neutron. Furthermore, the angular distribution of neutrons emerging from a given scattering interaction is assumed to have cylindrical symmetry about the incident direction. The double-valued region, i.e., neutrons of incident energy

$$\frac{Q(A+1)}{A} \leq E \leq \frac{QA}{A-1}$$

is processed using the center-of-mass method described in Sec. IV F. The main practical limitation of Eq. (12) is the determination of the number and values for Legendre expansion coefficients of the scattering angular distribution in the laboratory system. The number of terms required to represent an angular

distribution to a given accuracy is always at least as large as the number of center-of-mass system Legendre coefficients, and is substantially larger for light nuclei. Rather than completely reconstructing the angular distribution over the entire range (-1 to +1) and determining the number of terms required by examination of the fit in a linear least squares sense,[18] the scheme actually implemented in MINX is based on examination of the differential angular distribution at 0° and 180° (for which computation of Legendre polynomials simplifies considerably) with respect to its sensitivity to successive terms in the series expansion. The number of terms in the laboratory expansion is determined when the forward and backward (0 and 180°) scattering cross sections are reproduced to within a user-specified tolerance.

F. Calculation of Multigroup Transfer Matrices for Two-Body Interactions Using the Center-of-Mass System

In the double-valued region for discrete inelastic scattering, in the region of low effective mass near the inelastic threshold, and for light scatterers, the laboratory expansion described above becomes impossible or uneconomical. In such cases, MINX uses a direct numerical integration in the center-of-mass system. The elements of the group-to-group scattering matrix become

$$\sigma^{j}_{g'\to g} = \frac{\int_{E_{g'}}^{E_{g'-1}} dE'\sigma(E')N_j(E') \int_{\omega_{g-1}}^{\omega_g} \sum_k \frac{2k+1}{2} f_k^{CM}(E')P_k(\omega_c)P_j(\omega_L)d\omega_c}{\int_{E_{g'}}^{E_{g'-1}} N_j(E')dE'} \quad (15)$$

The integral over ω_c is performed by adaptive quadrature, and the energy integral is performed as in Sec. IV E. This alternate calculation is used whenever it takes more than 14 Legendre terms to describe the angular distribution in the laboratory frame.

G. Multigroup Neutron Transfer Matrix Formulation for Scattering Reactions in which the Outgoing Neutron Energy and Scattering Angle Are Uncoupled

The derivation of the expression for multigroup transfer matrices for processes in which the outgoing neutron energy and scattering angle are uncoupled is more straightforward than that required in Sec. IV E. The definition is

$$\sigma^{j}_{g'\to g} = \frac{\int_{E_g}^{E_{g-1}} \int_{E_{g'}}^{E_{g'-1}} N_j(E')\sigma_j(E'\to E)dE'dE}{\int_{E_{g'}}^{E_{g'-1}} N_j(E')dE'} \quad , \tag{16}$$

where

$\sigma^{j}_{g'\to g}$ = j^{th} Legendre component of the group-to-group matrix for scattering from group g' to group g,

$E', E_{g'}, E_{g'-1}$ = source energy E' in source group g' bounded by $E_{g'}$ and $E_{g'-1}$ (similarly for sink energy E),

$N_j(E')$ = j^{th} Legendre component of the neutron angular flux weighting function, and

$\sigma_j(E'\to E)$ = j^{th} Legendre component of the microscopic differential scattering cross section (note that fission and (n,2n) may be included within the scattering definition).

The differential scattering cross section may be represented explicitly as

$$\sigma(E'\to E, \underline{\Omega}'\to\underline{\Omega}) = m(E')\sigma(E')p(E'\to E)t(E',\omega_L) \quad , \tag{17}$$

where

$m(E')$ = multiplicity of the reaction,

$\sigma(E')$ = cross section for the reaction,

$p(E'\to E)$ = neutron energy distribution (probability) for scattering from E' to E within a differential energy bin dE,

$t(E',\omega_L)$ = angular distribution of neutrons emerging from scattering,

$\sigma(E'\to E, \underline{\Omega}'\to\underline{\Omega})$ = differential scattering cross section for neutrons

Note that for the reactions under consideration, the energy distribution $p(E'\to E)$ is assumed to be completely separable from the angular distribution $t(E',\omega_L)$. Here, the angular distribution is also assumed to depend only upon the cosine of the scattering angle ($\omega_L = \underline{\Omega}'.\underline{\Omega}$). The formulation which follows is quite general in that it imposes no restriction on the order of scattering.

With these approximations to the differential scattering cross section, the Legendre component of the transfer matrix becomes

$$\sigma_j(E'\to E) = m(E')\sigma(E')p(E'\to E)T_j(E') \quad , \tag{18}$$

where

$$T_j(E') = \int t(E',\omega_L)P_j(\omega_L)d\Omega' \quad . \tag{19}$$

Substitution of Eq. (18) into Eq. (16) results in

$$\sigma^j_{g'\to g} = \frac{\int_{E_{g'}}^{E_{g'-1}} dE'\ N_j(E')m(E')\sigma(E')T_j(E')\int_{E_g}^{E_{g-1}} p(E'\to E)dE}{\int_{E_{g'}}^{E_{g'-1}} N_j(E')dE'} \quad . \tag{20}$$

The flexibility of ENDF/B permits each of the energy distributions $p(E'\to E)$, to be broken down into partial energy distributions $f_k(E'\to E)$ where each of the partial distributions can be described by different analytic representations

$$p(E'\to E) = \sum_k p_k(E')f_k(E'\to E) \quad , \tag{21}$$

with the fractional probabilities p_k summed over all k being normalized to unity. The secondary spectra $p(E'\to E)$ is normalized, such that

$$\int_0^{E'_{max}} p(E'\to E)dE = 1 \quad , \tag{22}$$

where E'_{max} is a function of the incident neutron energy (E'). If one defines

$$Z^k_j(E') \equiv m(E')\sigma(E')T_j(E')p_k(E')N_j(E') \quad , \tag{23}$$

and substitutes Eqs. (21) and (23) into Eq. (16), one obtains the expression for the multigroup transfer matrix which is evaluated numerically (because $f_k(E'\to E)$ is <u>not</u> separable in E and E')

$$\sigma^{j}_{g'\to g} = \frac{\sum_{k} \int_{E_{g'}}^{E_{g'-1}} dE' \; Z^{k}_{j}(E') \int_{E_{g}}^{E_{g-1}} f_{k}(E'\to E)dE}{\int_{E_{g'}}^{E_{g'-1}} N_{j}(E')dE'} \quad . \tag{24}$$

MINX evaluates Eq. (24) for all the types of File 5 representations.

H. Treatment of Fission Matrices and Spectra (Fission Chi)

The present version of MINX does not produce a full fission transfer matrix. Most existing reactor codes require the normalized fission spectrum, or Chi vector, defined by

$$\chi_{g} = \frac{\int dE' \int_{g} dE \; \nu(E')\sigma_{f}(E')\chi(E'\to E)\phi(E')}{\int dE' \nu(E')\sigma_{f}(E')\phi(E')} \quad , \tag{25}$$

where E' and E are the initial and final neutron energies, ν is the fission yield (from File 1 of the ENDF/B tape), σ_f is the fission cross section (from File 3), χ is the normalized fission neutron spectrum (from File 5), and ϕ is the neutron flux. This is clearly an application-dependent quantity due to its dependence on the flux at all energies. However, χ is often a slowly varying function over the most important range of incident energies; therefore, the multigroup χ can be approximated by

$$\chi_{g} \simeq \int_{g} dE \chi(E^{*}\to E) \quad , \tag{26}$$

where E* is some energy in the range of interest. This is a good approximation for fission reactor applications and has been widely used. MINX uses E* = 1 MeV.

The ENDF/B-IV files have a more sophisticated representation of the fission process than the earlier version. First, second, third, and fourth chance fission are represented explicitly by the (n,f), (n,n'f), (n,2nf), and (n,3nf) reactions. The spectra of fission neutrons from the last three reactions include a scattering type of energy dependence which improves the accuracy of the representation of fission at high energies. The current version of MINX only uses the MT18 energy spectrum.

V. CCCC OUTPUT FORMATS

The MINX code was written to provide multigroup constants for the interface system specified by the Committee on Computer Code Coordination.[11,23] The role of MINX in this system is made clear by Fig. 2. The CCCC ISOTXS (isotope cross section) and BRKOXS (self-shielding factors) files are generated in a fine group structure using MINX to process ENDF/B data. These files are combined into libraries and transmitted between installations using LINX and BINX.[33] If necessary or convenient, the multigroup sets can be collapsed to a coarser group structure using CINX.[34] Finally, the SPHINX[9] code is used to combine isotopes into macroscopic cross sections and to perform a space-energy collapse. The result is a set of few group cross sections suitable for use in a reactor design or operation calculation.

The CCCC Version III ISOTXS and BRKOXS output interface files are generated in the FOURC module. (The formats for these two files are listed in Appendix H[11,23] for reference.) This module reads cross sections, f-factors, fission chi vectors (all from the MULTIG stored file) and transfer matrix elements (from the MULTIX file), sums and reorders them, and computes associated pointers, bandwidths, etc. Quantities such as isotope name and fission energy release which are not available from MINX must be entered by the user.

The following restrictions and variations should be noted:

Storage. FOURC requires a storage area for matrices of $\ell n(n+1)/2$ words where ℓ is the number of Legendre terms and n is the number of groups. This labeled COMMON area is dimensioned for 12 000 words (this is enough for P_4 matrices with 68 groups). It can easily be increased if a large machine or extended core storage is available to the user.

Blocking. Transfer matrices are sub-blocked so that there is a record for each final energy group containing elements for all Legendre orders and all initial energy groups.

Cross Sections. The elastic, inelastic, (n,2n), and elastic removal cross sections are obtained by summing the final energy groups for the associated matrix and dividing by the multiplicity. All other cross sections are obtained from MULTIG.

F-factors. The "total" f-factor contains the current weighted value from MINX, and the "transport" f-factor contains the value computed in MINX (see Sec. IV D).

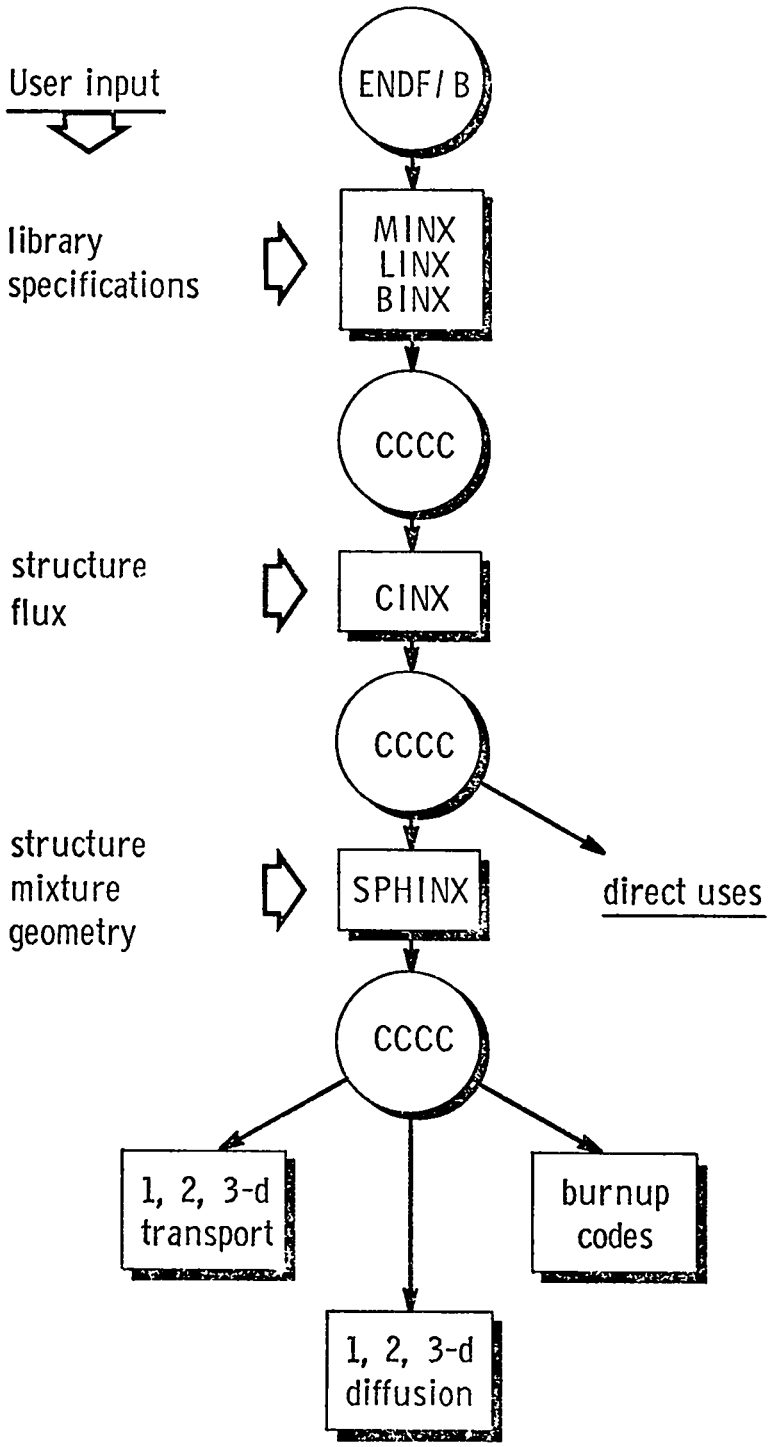

Fig. 2. Outline of CCCC interface system for generating multigroup constants for fast reactor analysis.

Chi. Set chi vectors or matrices, or isotope chi matrices, are not provided. The isotope chi vector was computed in MINX by an approximate method (see Sec. IV H).

Potential Scattering. The potential scattering is obtained from MULTIG. It was computed using the full spin-dependent formula for σ_p and may not be meaningful above the resonance range.

Energy Release Parameters. Values quoted for the average energy released in fission (EFISS) were obtained through a linear interpolation and extrapolation of data quoted by M. F. James[35] for four fissionable isotopes. This procedure resulted in uncertainties which are probably in the vicinity of 2%. The calculation of the energy released through neutron capture (ECAPT) was performed by adding the Q-value[36] of the initial capture to the energy released through the eventual decay of the residual nucleus to a stable isotope. Dominant modes of decay and their associated energies were taken from the Table of Isotopes.[37] Calculation of the average energy released locally in beta decay (i.e., the energy not associated with the neutrino) was performed according to the formula

$$\overline{E}\,(\beta) = 0.511 \langle W-1 \rangle \quad , \tag{26}$$

where

$$\langle W-1 \rangle = \frac{Wo^6 - 2Wo^5 + 5Wo^2 - 6Wo + 2}{2Wo^5 - 20Wo^2 + 30Wo - 12} \quad , \tag{27}$$

and

$$Wo = \frac{E_{max}(\beta)}{0.511} + 1 \quad . \tag{28}$$

In the above formulation, $E_{max}(\beta)$ is the maximum energy available to the electron in the decay. All energies are given in MeV. Energy values for EFISS and ECAPT were quoted in joules where the conversion factor is,

$$1 \text{ MeV} = 1.602 \times 10^{-13} \text{ J} \quad .$$

Other Output Formats. It should be noted that the MULTIG and MULTIX internal interface files contain all the group constants computed by MINX in simple

binary records. Therefore, special installation-dependent formats can be constructed by replacing the FOURC module with a new program designed to read MULTIG and MULTIX. No modifications to the main body of MINX should be required.

VI. MINX INPUT PREPARATION

The user's input cards are prepared as described below. Note that some sets of cards use the ENDF/B BCD formats.[1]

Card Type 1 (20A4) "Title"

TITLE - Descriptive information.

Card Type 2 (6I5) "Control"

MAT1 - Lower ENDF/B MAT number to be processed.

MAT2 - Upper ENDF/B MAT number.

NOTAPE - Start and restart options.

= 0, start from beginning using only ENDF/B tape on unit 20.

= 1 restart from existing PENDF tape on unit 21 and ENDF/B on unit 20.

= 2 restart from partially completed PENDF on unit 12 and ENDF/B tape on unit 20 (restart card required).

LPRINT - Print control (0 max, 1 min).

NTMP - Number of temperatures (in addition to 0 K), NTMP $\geq$ 1.

NSIG - Number of background cross sections (in addition to infinity), NSIG $\geq$ 1.

Card Type 3 (I5,2E10.0) "Restart"

Only read if NOTAPE=2.

NDONE - Number of temperatures successfully completed (counting 0 K).

RESLO, RESHI - Upper and lower energy limits for Doppler thinning. Normally limits of resolved resonance range.

Card Type 4 (4E10.0) "Tolerances"

ERR1 - Resonance reconstruction tolerance (fractional).

ERLIN - Linearization tolerance (fractional).

ERTHN - Thinning tolerance (fractional).

ERINT - Adaptive integration tolerance (fractional).

Card Type 5 (6E10.0) "Temperatures"

TB - Temperatures in degrees Kelvin (0 K is done automatically).

Card Type 6 (6E10.0) "Sigma Zeroes"

SIGPT - Background cross sections in barns (infinite is done automatically).

Card Type 7 (16I5) "Options"

JTERMS - Number of Legendre orders for scattering matrices ("1" means "P_0" only).

LTERMS - Number of Legendre orders for a user-supplied weight function.

IGRID - Energy group structure.

= 1, read in by user.

= 2, CSEWG 239 group + dump group.

= 3, GAM-II 100 group.

= 4, SAND-II 620 group.

= 5, LASL 30 group.

= 6, GAM-I 68 group.

= 7, RRD 50 group.

IWT - Smooth weight function.

= 1, constant.

= 2, 1/E.

= 3, thermal + 1/E + fission.

= 4, read in by user.

NENPTS - Number of energy points in group structure if IGRID = 1 (number of groups plus one).

NEWT - Number of energy points in weight function if IWT = 4.

NOREAC(1) - Selects reactions to be processed.

= -1, reactions specified for CCCC-III format, (also triggers CCCC output processing).

= 0, everything on ENDF/B tape.

= N, the 2 $\leq N \leq$ 50 reactions read in below (MT1 and MT2 must be processed).

ICHOP - If not zero, reduce group structure to a 15 MeV maximum.

Card Type 8 (16I5) "Reactions"

Only read if NOREAC(1) is greater than zero.

NOREAC(N) - Reaction MTs to be processed, include MT1 and MT2 first.

Card Type 9 (LIST) "Group bounds"

Only read if IGRID = 1.

NENPTS - Group energies as an ENDF/B LIST record: (44X,I11/(6E11.0)).
ENPTS Increasing or decreasing order.

Card Type 10 (TAB1) "P_0 weight"

Only read if IWT = 4 and LTERMS = 1.

ENFLX
FLUXL - Tabulation of P_0 weight function in ENDF/B TAB1 form (see Ref. 1 for detailed format). Low energy to high.

Card Type 11 (TAB2/LIST) "P_n weights"

Only read if IWT = 4 and LTERMS > 1.

ENFLX
FLUXL - Tabulations of P_0, P_1,... weights using a TAB2 record with slave LIST records for each energy (see Ref. 1 for detailed format). Low energy to high.

Card Type 12 (4E11.0) "Analytic Weight"

Only read if IWT = 3.

TB - Temperature (eV) for thermal Maxwellian.

EB - Break energy (eV) between Maxwellian region and 1/E region.

TC - Temperature (eV) for fission spectrum.

EC - Break energy (eV) between 1/E region and fission spectrum region.

Card Type 13 (12A6) "Set ID"

Only read if NOREAC(1) = -1.

HSETID - Descriptive label for CCCC files.

Card Type 14 (5A6,2I6,2E12.0) "CCCC data"

Only read if NOREAC(1) = -1. See Ref. 21 for detailed specifications of these parameters.

HUSE(2) - User identification.

HISONM - Isotope name.

HABSID - Absolute isotope label.

HMAT - ENDF/B material number.

IVERS - Version number for CCCC file.

KBR - Isotope classification.

EFISS - Fission energy release (W-Sec/Fiss).

ECAPT - Capture energy release (W-Sec/Capt).

Most of the card specifications are self-explanatory or will be made clear by the sample input decks below. Since the production of the pointwise data library (PENDF) is expensive, it is important to understand the restart options. The user should always arrange to save the contents of unit 21. It can be used with NOTAPE = 1 for subsequent multigroup processing with different conditions.

Recovery from "time limit" during Doppler broadening can be obtained by using NOTAPE = 2 along with card type 3 if unit 21 was saved.

Deck 1. 50 group CCCC library run from scratch.

```
$JOB(NAME=T2MACFARL,CL=J,AC=T02NJOY,JA=95320146302,LC=400000,
$TPL=70,TL=2M,PR=21)

J=235 FOR MINX 50-GROUP ENDF/B-IV LIBRARY.
 1261 1261    0    0    3    6
.005       .002       .002       .001
300.       900.       2100.
10000.     1000.      100.       10.        1.         .1
    4    1    7    3    1    1   -1    0
        .025          .1        1.4E6     .8208E6
J=235 FOR MINX 50-GROUP ENDF/B-IV LIBRARY.
T2LASLMINX    J235  J235  1261     1      2   3.2362-11   1.7684-12
```

Deck 2. Restart from existing PENDF tape.

```
J=235 FOR MINX 50-GROUP ENDF/B-IV LIBRARY.
 1261 1261    1    0    3    6
```

Continue as in deck 1.

Deck 3. Restart from partial PENDF tape to add an additional temperature.

```
J=235 FOR MINX 50-GROUP ENDF/B-IV LIBRARY.
 1261 1261    2    0    4    6
    4         1.        92.
.005       .002       .002       .001
300.       900.       2100.      5000.
```

Continue as in deck 1.

Deck 4. User defined group structure and weight function starting from existing PENDF tape.

```
J=235 FOR SPECIALLY WEIGHTED 11 GROUP LIBRARY.
 1261 1261    1    0    3    6
.005       .002       .002       .001
300.       900.       2100.
10000.     1000.      100.       10.        1.         .1
    4    1    1    4   12    5   -1    0
                                                    12
         1-5        1-3        1-1         1.       1+1        1+2
         1+3        1+4        1+5        1+6       1+7        2+7
                                                     2          5
           2          5          5          2
         1-5        1+5        1+5        1-5       3+5        2-6
         1+6        3-6        2+7        3-6
J=235 FOR SPECIALLY WEIGHTED 11 GROUP LIBRARY.
T2LASLMINX    J235  J235  1261     1      2   3.2362-11   1.7684-12
```

VII. CODING DETAILS

The MINX code is large and complex (almost 15 000 source statements and 200 subroutines), but an attempt has been made to keep it understandable by using standard FORTRAN, modular organization, and many comment cards. Some features of the coding of special interest to the user are discussed below.

A. Non-Fatal Diagnostics

The user should note the following messages:

"NOT CONVERGED FROM [E_1] TO [E_2] [n] POINTS GENERATED" From RESEND Code cannot add more than 500 points between any two resonance centers. Expected accuracy will not have been achieved.

"TEST FOR 5 DECIMAL PLACES REJECTED [n] POINTS" From RESEND. The BCD ENDF/B formats used in MINX allow for five figures after the decimal. If two energy values are identical to this precision, one is removed (example: ^{238}U). Expected accuracy will not have been achieved.

"NEG SIGMA SET TO ZERO IN LINIZE [E] [σ] [MT]" From LINIZE. Because of inadequate single-level Breit-Wigner representations for elastic scattering resonances, negative cross sections are possible in the interference dips below each resonance (example: ^{238}U). MINX sets these negative cross sections to zero.

"ENERGY [n] NOT CONVERGED IN CONVTD" From CONVTD. It was not possible to represent the angular distribution at the indicated energy with a Legendre expansion of order 20. Expansion truncated.

B. Fatal Error Exits

There are many conditions that may require MINX to halt execution. These error exits are numbered as described below. All exits are made through the ERROR subroutine.

Error	From	Definition
2	Point 3	Available storage exceeded
3	Point 3	Available storage exceeded
4	Point 4	Available storage exceeded
5	Point 5	Available storage exceeded
6	Point 6	Available storage exceeded
7	Point 7	Available storage exceeded
8	Point 8	Available storage exceeded
9	Point 9	Available storage exceeded
10	UCPRC	Available storage exceeded

11	UCPRC	Available storage exceeded
23	UNIND	Unionization pointer error
110	ECSI	Interpolation code out of range
133	TERP1	Interpolation code out of range
134	TERP1	Zero or negative value cannot be interpolated by logs.
140	DBTERP	Unable to find interpolation code
152	UCPREP	No fission cross section present
181	ISLIN1	X1 is greater than X2
182	ISLIN1	XM is less than X1
183	ISLIN1	XM is greater than X2
201	RDBW	Exceeded available storage
202	RDUNR1	Exceeded available storage
203	RDUNR2	Exceeded available storage
204	RDNORP	Exceeded available storage
205	RDAA	Exceeded available storage
206	CSAA	Illegal LI value
297	CSMLBW	Illegal J value
298	CSMLBW	Too many J values required for this L
299	CSMLBW	Statistical sum incorrect
300	RPTAB	Unable to find interpolation code
315	GRATE	Interpolation table incorrect
500	COMBR	Interpolation table incorrect
516	TMF1	Illegal value of LNU in File 1
526	GETIN	Cannot find desired point
537	TERPO	Invalid interpolation scheme or X out of range
582	RANGE	Cannot find desired point
747	GETSIG	End-of-file on unresolved tape
810	CONT	Requested record incorrect or missing
815	TMAT	Unable to find requested material on tape
820	WTFN	Energy range error
843	GETFK	Interpolation table error
850	GETWFJ	Interpolation table error
910	XMBAN	CCCC matrix storage exceeded

Error 910 can be corrected by enlarging /MATRIX/ in XMBAN on IBM machines or moving it to Large Core Memory (LCM) on CDC 7600's.

C. Subroutine Identification

Subroutine	Function
MINX	- The program driver which calls various overlay structures. Core requirement and page size initialization is also done.
ERROR	- Error exit routine. Forces system exit and returns last location read from ENDF tape. Contains list of all error messages in MINX.
BANNER	- Write MINX banner on listing.
RUINA	- Reads first part of user's input.
CMEND	- Copies up to and including the MEND record of an ENDF/B data tape; will read and write or only read (BCD only).
CFEND	- Copies to the end of an ENDF/B data file; will read and write or only read (BCD only).
MEND	- Reads ENDF/B records and will skip to the next MEND card (BCD only).
FEND	- Reads ENDF/B records and will skip to the next FEND card (BCD only).
CONTIN	- Reads in one ENDF/B control record (BCD only).
CONTOT	- Write out one ENDF/B control record (BCD only).
CXFP	- Converts floating point numbers to maximum ENDF/B permitted significant digits.
SEND	- Copies one ENDF/B section from one unit to another (BCD only).
REED	- Binary reading subroutine for all CCCC interface files.
RITE	- Binary writing subroutines for all CCCC interface files.
STOW	- Storage of one vector into another at a specified starting address.
ISLIN1	- Used to linearize all pointwise File 3 data. The routine finds for a given interpolation type the point XM between X2 and X1 at which the interpolate differs most from a linear-linear interpolate.
TERP1	- Used to interpolate for one point using ENDF/B interpolation laws.

OVERLAY 1,0 (First Phase of Pointwise Cross Section Generation)

Subroutine	Function
RESEND	- Generate infinitely dilute unbroadened point cross sections in the ENDF/B format. Pointwise cross sections are produced by combining the File 2 resonance parameter data with the File 3 background cross-section data. The combining and generation of the pointwise data is done to within a specified tolerance. Uses two secondary overlays.
DUMFIL	- Write a dummy File 1 and File 2 for ENDF/B.
ZEROC	- Zeroes out an ENDF/B control record.

OVERLAY 1,1 (Second Phase of Pointwise Cross-Section Generation)

Subroutine	Function
PROF2	- Processes ENDF/B File 2 data (resonance parameters) and stores the calculated cross sections on a scratch unit.
SIGMAP	- Computes pointwise potential scattering cross section which is written on PENDF tape as MT285.
RDFIL2	- Reads the ENDF/B File 2 data and stores parameters in blank common.
SIGMA	- Calculates the cross section at an energy point from resonance data stored in blank common.
DUMPCS	- Dumps N entries from vector E and array CS and updates the next starting location.
RDBW	- Reads in one section consisting of resolved Breit-Wigner parameters. Also used for single, multilevel or Reich-Moore data.
RDNORP	- Reads one ENDF/B section which contains no resonance parameters.
RDUNR1	- Reads one ENDF/B section consisting of unresolved (energy-independent) parameters.
RDUNR2	- Similar to RDUNR1, only reads in the energy-dependent unresolved resonance parameters.
CSNORP	- Calculates potential scattering cross section for an isotope without resonance parameters.
CSSLBW	- Calculates single-level Breit-Wigner cross section at given energy and for one section.
CSMLBW	- Calculates multilevel Breit-Wigner cross section at given energy and for one section.
CSUNR1	- Calculates unresolved resonance region cross section (infinite dilution and 0 K) for single-level Breit-Wigner (energy-independent) parameters.
CSUNR2	- Same as for CSUNR1 only for energy-dependent parameters.
FACTS	- Calculates penetration and shift factors.
FACPHI	- Calculates phase shift.
UNFAC	- Calculates the penetrability factor and phase shift.
GNRL	- Calculates fluctuation integrals for unresolved resonances.
INTERF	- Interpolates fission widths for unresolved representation.
INTER	- Interpolates energy-dependent unresolved resonance parameters.
MESH	- Prepares a table of energy vs cross sections based on an optimum mesh. The mesh is generated starting from a fixed set of nodes and sub-dividing intervals until convergence is obtained in each interval. (See write-up for more specific details on convergence.)

ORDER	- Sorts N elements of an array into ascending floating point order.
RDAA	- Reads one section of resolved Adler-Adler parameters and stores in blank common.
CSAA	- Calculates the multilevel Adler-Adler cross sections at energy point for one section.

OVERLAY 1,2 (Final Phase of Pointwise Cross-Section Generation)

Subroutine	Function
PROF3	- Control Program for combining ENDF/B File 3 data with the resonance cross sections.
MKSECT	- Produces a section by processing resonance data into a TAB1 format. Routine is used when there is no background.
RDTABX	- Reads the first part of a TAB1 record including interpolation law.
PRSECT	- Write out a File 3 section in ENDF/B format.
COMBR	- Combine resonance cross sections with File 3 backgrounds.
STORS	- Used to store energy and cross section points on a scratch unit.
FINDX	- Logical retrieval routine for summed data.
FINDB	- Logical retrieval system for File 3 background data.
FINDR	- Logical retrieval system for resonance data.
LOADR	- Logical page loader for resonance data.
LOADB	- Logical page loader for File 3 data (BCD only).

OVERLAY 2,0 (Doppler Broadening and Linearization)

Subroutine	Function
SIGMA1	- The control program for Doppler broadening and linearization of the data. All data is linearized to specified tolerance prior to any Doppler broadening.
FILE3	- Used to load data into core and Doppler broaden it one page at a time. (In Doppler broadening, a page is defined as 1002 or fewer points).
TABFIN	- Used to copy a section of broadened and/or thinned data from core to result output file.
THINB	- Used to thin broadened data to within a specified tolerance. If criteria is zero, no thinning is performed.
BROADN	- Used to exactly Doppler broaden the cross sections at a portion of the energies corresponding to the original cross section.
FUNKY	- Defines functions which appear in Doppler broadening calculations.
ERF	- Calculates error function for specific value.
ERFC	- Calculates complimentary error function for specific value.

HUNKY - Defines functions which appear in Doppler broadening calculation.

RDTABX - Reads first part of TAB1 record including the interpolation law.

LINIZE - Linearizes ENDF/B data to the material end (MEND) card.

GETIN - Retrieves MT data pairs from current section being linearized.

OVERLAY 3,0 (Unresolved Calculation)

Subroutine	Function
UNRESR	- Control of unresolved resonance region. Computes unresolved resonance cross sections and stores on tape for retrieval by GETSIG.
RDUNF2	- Reads unresolved resonance parameters from File 2 of ENDF/B tape.
RDUNF3	- Reads background cross sections from File 3.
UNRESL	- Computes effective cross sections in the unresolved region using ETOX method.
UNFAC	- Calculates the penetrability factor and phase shift.
INTERF	- Interpolates fission widths for unresolved representation 1.
INTER	- Interpolates energy-dependent unresolved resonance parameters.
QUICKW	- Used to calculate ψ and χ line shape functions.
AJK	- Calculates J and K integrals (see Sec. IV-E).
WTAB & W	- Generates table of complex probability integral W.

OVERLAY 4,0 (Main Control of Group Averaging of Cross-Section Information)

Subroutine	Function
TERROR	- Main driver and control for group averaging of pointwise cross section and calculation of all transfer matrices.
POINT1	- Used to calculate a set of flexible dimension pointers.
RUINB	- Used to read in the users input parameters for group averaging and transfer matrix calculations. Also defines several I/O units used in group averaging.
ECSI	- Computes integral of y(x) (ENDF/B slave routine).
GRATE	- Integrates a TAB1 ENDF/B function (ENDF/B slave routine).
LIST	- Reads in an ENDF/B LIST record and stores record (ENDF/B slave routine).
TAB2	- Reads in an ENDF/B TAB2 record.
TA2FX	- Used to read a TAB2 record which has been written in floating point.
CONT	- Reads and checks six types of control records. Also notes information on scratch file while looking for information (modified ENDF/B slave routine).

TAB1	- Used to read an ENDF/B TAB1 record (modified ENDF/B slave routine).
HOLL	- Used to read Hollerith information on ENDF/B tape. Reads one record (card) and then write out. Does not store single record (card) information (modified ENDF/B slave routine).
TABFIX	- Used to read an ENDF/B TAB1 record which has been written in floating point.
TMAT	- Used to search and position (ENDF/B slave routine).
TMF1	- Used to read an ENDF/B File 1 information (ENDF/B slave routine).
TMF3	- Used to read information in File 3 of an ENDF/B tape for a particular reaction (MT) type (ENDF/B slave routine).
TPOS	- Used to position ENDF/B tape to a particular file (MF) (ENDF/B slave routine).
RUSEG	- Used to read in group structure or to structure the standard group structures available to user.
XL15	- Used to squeeze part of group structure above 15 MeV into equal small groups below 15 MeV. Used on option only.
WTFN	- Used to read in an arbitrary weight function as given by the user.
POINT2	- Used to establish pointers for flexible dimensioning of program.
POINT3	- Used to establish pointers for flexible dimensioning of program.
RITFL	- Used to flag write option. If on, then various ENDF/B files will be written on BCD scratch files.
POINT4 POINT5 POINT6 POINT7	- Used to establish pointers for flexible dimensioning of program.
SIMPSN QNC7	- Adaptive integration routines, two are used in cases of double integrations.
READF	- Used to read in the angular distribution functions of the secondary neutrons and store them in the laboratory reference system.
LABF	- Used to calculate transformation matrix (elastic only) if required, and to perform the necessary operations to get secondary angular distributions in the laboratory system; also, stores the laboratory angular distributions.
GENTM	- Used to calculate 1/A expansion to a specified tolerance in addition to finding largest order of angular expansion.
TT BB	- Used to generate data for transformation matrix.

CONVTD	- Used to convert angular distributions which are given as probabilities to Legendre coefficients. Calculation is done to within a specified tolerance by use of least squares criteria.
ARGE	- Used to calculate integrands employed in testing the convergence of calculating Legendre coefficients from probability distributions.
TERPO	- Used to interpolate within a given vector.
GETESX	- Finds the particular cross section for a specific energy and interpolation code.
GETFK	- Finds the particular Legendre coefficient for a specific energy and interpolation code - laboratory coefficient.
GETCFK	- Finds the particular Legendre coefficient at a specific energy and interpolation code - center-of-mass coefficient.
GETWFJ	- Finds the particular weight function at a specific energy.
ISRCH	- Binary search routine.
PTWT	- Used to determine weight function for constant, 1/E, and 1/E + fission + thermal.
CDEF	- Used to calculate 1/E + fission + thermal.
STORE	- Used to store cross sections and interpolation information.
RPTAB	- Used to read in one page of data from ENDF/B tape.
UNIND	- Used to unionize data in the integration procedure.
UNINIT	- Used to initialize parameters for unionization of data in integration procedure.

OVERLAY 4,1 (Smooth Averaging)

Subroutine	Function
SMOOTH	- Control program for the smooth averaging and f-factor calculation of ENDF/B pointwise cross sections
GRUPXS	- Routine initializes parameters and pointers, monitors the flow of calculation, editing of calculations and proper storage of calculated cross-section information
INTXS	- This routine reads in the pages of data required for calculation. Once the proper pages are in core, the corresponding integration limits are determined, and the data for the limits is unionized on the energy mesh.
GPXSEC	- Used to calculate the integrand (numerator and denominator) for the smooth averaging of cross-section information
GETSIG	- Used to interpolate for reaction cross section after obtaining the correct cross-section points. Uses unresolved cross section if needed and will retrieve unresolved data from tape as required.

RANGE - Used to find the index for the first point in a vector which is greater than or equal to some input point. Keeps track of where it was in the vector.

MTNAME - Editing routine which puts proper labels and reaction type information for each reaction process.

OVERLAY 4.2 (Elastic and Discrete Inelastic Transfer)

Subroutine	Function
TRANFR	- Main driver for the elastic and discrete inelastic transfer calculation. Controls input of cross-section information and positioning of the ENDF/B tape.
INTWF	- Computes the integral of the input weighting function which is used in the denominator of the transfer cross-section calculation.
YJLZJL	- Calculates integral of $P_K(\omega)P_J(\omega)d\omega$ over interval A to B (see main write up).
AFKCM	- Calculates the inner integrand for center-of-mass expansion whose data is given in center-of-mass.
GGESXS	- Heart of the group-to-group elastic scattering calculation. Reads in required pages of cross section, performs necessary operations and output transfer cross sections onto MULTIX.
GETKTR	- Used to determine the largest number of angular terms required in the angular expansion for a particular energy group.
GGISXS	- Heart of the group-to-group discrete inelastic scattering calculation. Reads in required pages of cross sections, performs necessary operations, and outputs transfer cross sections onto an interface tape.
FGIN	- Calculates Legendre coefficients in the laboratory system for discrete inelastic. Employed if original angular distributions are given in center-of-mass system.
ARG	- Calculates the integrand for the elastic group-to-group calculation. Does calculation for each energy specified by the adaptive integration scheme.
ARIND	- Same as ARG only for discrete inelastic transfer.
UXFCM	- Used in discrete inelastic system transformation. Multiplies the center-of-mass Legendre coefficients by the transformation matrix.
LABEXP	- Determines a quasi-optimal number of angular expansion terms required in the group-to-group calculation (see Sec. IV-E).
GETP	- Used by XPAN to find the correct Legendre polynomial (correct order and value).
XPAN	- Calculates the various integrands required by LABEXP in determining the number of terms required in angular expansion.
STORE	- Used to store data from one vector to another.

SKINTS - Calculates the maximum energy loss during discrete inelastic scattering.

CRITS - Calculates critical points for discrete inelastic scattering to a particular final group (the inverse of SKINTS).

OVERLAY 4,3 (Calculation of Continuum Transfer Matrices)

Subroutine	Function
CONTSC	- Control of continuum scattering multigroup transfer calculation.
UCPREP	- Reads the ENDF/B tape and finds the various continuum processes. MINX processes all continuum processes that are on the ENDF/B tape.
UCPRC	- Reads in File 4 and File 5 information for continuum and calls routines which calculates pointers and store information.
POINT8	- Calculates pointers for storing of probability table.
POINT9	- Calculates pointers for storing interpolation tables.
POINTA	- Calculates pointers for storage of scattering functions when they are not analytic models.
STLF11	- Storage and editing routines for various continuum laws.
STLF12	
STRPM1	
SFPAR	
STLF13	
STLF31	
STLF51	
STLF71	
STLF53	
STLF72	
STLF91	
STLF92	
STLF10	
UCCAL	- Heart of group-to-group continuum scattering calculation. Reads in required pages of cross section, performs necessary operations and outputs transfer matrices.
SOURCE	- Calculates the integrand of the transfer calculation at the energy specified by adaptive integration scheme at the correct secondary law.
UNLF1	- Control of law 1 - seeks correct function value for input incident energy.

QKCK	- Used in law 1 to calculate the limit of final energy which will be later used to see if in correct energy region.
UHLP1	- Used in law 1 to generate a function for given incident energy by use of surrounding data.
GEE	- Calculates inner integrand for the law 1 calculation.
GETGP	- Fetches correct probability value for incident energy value.
DBTERP	- Used by law 1 to perform double interpolation.
UNLF3	- Seeks correct function value for input incident energy for law 3. (Obsolete)
UNLF5	- Calculates correct function value for input incident energy for law 5.
UNLF7 UNL7A	- Calculates correct function value for input incident energy for law 7; UNL7A will perform the inner integral for this law.
UNLF9	- Calculates correct function value for input incident energy for law 9.
UNLF10	- Calculates correct function value for input incident energy for law 10.
STOOR	- Stores data from one vector to another.
EDITUC	- Upon option this routine will edit secondary energy distribution data.
CALPT	- Increment various pointers used to store data.
GETDAT	- Fetches correct secondary distribution data if such is not analytic.
LOC	- Finds the correct row, column index for matrix stored as a vector.
CSUM	- Calculates column sum of matrix.

OVERLAY 5,0 (CCCC Output)

Subroutine	Function
FOURC	- Primary control of CCCC output files (ISOTXS and BRKOXS).
ESTRC	- Restores energy grid to obtain more core; stores at beginning of blank common.
FCSX	- Reads in required cross sections and f-factors.
XINCOM	- Used to combine transfer matrices and to determine band widths for all scattering processes and to store all data in proper CCCC structure.
XMBAN	- Used to clear, store, and write various scattering matrices for the CCCC format.
SUMCIM SUNCIM	- Adds constants to specified elements of a vector.
CISFC	- Used to set up file control of ISOTXS file.

CISFD - Used to set up file data for ISOTXS file.

CIFID - Used to set up file identification for ISOTXS and rewind I/O units.

CISIL - Used to write isotope control and group-dependent data files for ISOTXS.

CISXS - Used to set up principal cross-section file for ISOTXS.

CISSB - Control routine for writing ISOTXS sub-scattering matrix blocks.

LOC - Computes a vector subscript for an element in a matrix.

GPXSX - Saves group structure for BRKOXS file.

CISOTX - Main control of structuring and writing ISOTXS file.

CBRKXS - Similar to CISOTX except for BRKOXS file.

BRFID - Used to set up file identification for BRKOXS and rewind I/O units.

BRFC - Used to set up file control for BRKOXS file.

BRFD - Used to set up file data for BRKOXS file.

BRSSF - Used to set up self-shielding factors for BRKOXS file.

BRSSFR - Used to read in self-shielding factors

XDVX - Rearrange vector from low-to-high to high-to-low.

SSFS - Store the self-shielding factors from a vector to a matrix.

BRXS - Read in cross sections for BRKOXS file.

WOT - Prints 1-, 2-, or 3-dimensional arrays.

WOT8 - Prints up to 8 one-dimensional arrays.

WOTI - Prints 1-, 2-, or 3-dimensional integer arrays.

PISOTX - Controls printing of the ISOTXS file.

PIFID - Rewinds units necessary to edit ISOTXS file and writes out identification file.

PBFID - Similar to PIFID only for BRKOXS file.

PBRKXS - Controls printing of BRKOXS file.

D. I/O UNIT USAGE BY OVERLAY

(1,0) RESEND

*20 NIN - BCD ENDF/B input tape.

*12 NOUT - BCD ENDF/B output tape with reconstructed resonances.

3 NSCRR - BIN scratch file of resonance cross sections.

4 NSCRS - BIN scratch file used in summing resonance and background cross sections.

(2,0) SIGMA1

*12 - BCD ENDF/B tape to be broadened (can be RESEND output or previous PENDF tape).

*21 - BCD PENDF output tape.

3 NSCRR - BCD scratch tape used for restart and bootstrap.

9 SCR - BIN scratch tape used in linearization and broadening.

(3,0) UNRESR

*20 NIN - BCD ENDF/B input tape.

* 8 NSCR - BIN output tape for unresolved resonance cross sections.

(4,1) SMOOTH

*21 - BCD PENDF input tape.

* 8 - BIN input tape of unresolved cross sections.

*18 MULTIG - BIN output tape for multigroup cross sections and f-factors.

3 MULETH - BCD scratch file for point elastic cross sections.

4 NSCRS - BIN scratch file for point total cross sections.

9 I09 - BIN scratch file for $\sigma_o = \infty$ multigroup cross sections for computing f-factors.

16 I16 - BIN scratch file for multigroup total cross sections.

(4,2) TRANFR

*21 - BCD PENDF input tape.

*17 MULTIX - BIN output tape for multigroup matrices.

3 I03 - BCD scratch tape for FILE3.

4 I04 - BCD scratch tape for FILE4.

9 I09
10 I010 - BIN scratch files used for paging.

(4,3) CONTSC

*21 - BCD PENDF input tape.

*17 MULTIX - BIN output tape for multigroup matrices.

*18 MULTIG - BIN output tape for multigroup cross sections (used for fission chi).

3 I03 - BCD scratch tape for FILE3.

4 I04 - BCD scratch tape for FILE4.

9 I09
10 I010 - BIN scratch tape used for paging.

(5,0) FOURC

*17	MULTIX	- BIN input tape for multigroup scattering matrix elements.
*18	MULTIG	- BIN input tape of multigroup cross sections, f-factors, and fission chi.
*1	ISOTXS	- BIN output tape for CCCC-III ISOTXS interface.
*2	BRKOXS	- BIN output tape for CCCC-III BRKOXS interface.
3	I03	- BIN scratch file used to rearrange BRKOXS cross sections.
4	I04	- BIN scratch tape for scattering bandwidths.
8	I08	- BIN scratch tape for ISOTXS cross sections.
9	I09	- BIN scratch tape of N2N cross section in ISOTXS and group bounds in BRKOXS.
10	I010	- BIN scratch tape for scattering matrices.
16	I16	- BIN scratch tape for BRKOXS cross sections and f-factors.

E. IBM Conversion and Implementation

The primary purpose of this section is to provide the IBM 360 user with useful information concerning conversion and implementation of the IBM version of the MINX code. In addition, some observations on significance problems are given with the hope that the programming experiences at ORNL will aid the effective use of the code at other installations.

In an attempt to expedite time consuming translation problems which result when computer programs are imported, the MINX code was developed with the requirement that it be as machine independent as possible and that it be made operational on at least two large computers. The following principles were used:

1. The only Hollerith delimiter used is "nH".
2. Hollerith constants are defined in DATA statements only.
3. Hollerith variables are limited to either four characters (ENDF convention) or six characters (CCCC convention). In the latter case, these variables are identified for changing to double precision on a "C IBM DOUBLE ..." card. Correct word counts are assured by changing the "MULT" parameter (Ref 21) from 1 to 2 (search for "C IBM MULT = 2").
4. No labeled COMMON has the same name as a program or subroutine.
5. Only standard FORTRAN-IV has been used.
6. Machine-dependent features such as Large Core Memory (LCM) storage or callable system routines have been avoided.
7. Memory requirements have been limited so that the code requires less than 50 000 words to execute.

Some system-dependent features could not be eliminated. These include the CDC overlay commands and the LASL date, time-of-day, and CP-time calls. They can be replaced by local equivalents.

A third class of machine dependent changes is required to permit accurate calculations on short-word-length machines. Since significance problems require a large programming effort to resolve, a summary of precision problems encountered to date will be given to help focus on those aspects of the multigroup calculation that may cause future trouble. Significance problems found include:

1. Selection of energy grid during pointwise reconstruction of ENDF data from resonance parameters.
2. Linearization for materials with lots of structure.
3. Computation of inner integration limits for elastic and discrete inelastic transfer matrix algorithms.
4. Evaluation of inner integral for center-of-mass expansion.
5. Evaluation of inner integral during continuum inelastic transfer matrix calculation. This applies to energy distributions represented by laws 7 and 9.

The MINX code has been implemented on the IBM-360/91 and IBM-360/195 using the IBM OS 360 operating system with the FORTRAN H compiler. In order to reduce main storage requirements, the overlay feature of the linkage editor is utilized. About 250k bytes of storage is required for the code. The CCCC interface option dictates the amount of common storage required for a problem. The following expression can be used to approximate common storage requirements:

$$10\ 000 + NENGPS*(NENGPS-1)+*TERMS/2$$

where NENGPS is the number of groups and JTERMS is the number of Legendre scattering terms (order +1). A 50-group problem will require about 330k bytes of core storage on an IBM machine.

The IBM version of MINX including the overlay structure (assignments of subroutines and common blocks) is available as a separate package.

VIII. VALIDATION AND SAMPLE PROBLEMS

A large and complex code like MINX can never be error-free. However, it is possible to minimize errors for the most common applications by (1) running a wide variety of cases, (2) testing against other similar codes, and (3) using the data to calculate benchmark systems. With regard to the first point, the LASL version of MINX has successfully processed every isotope in the ENDF/B-IV general purpose files and some isotopes from Version III (see Secs. VIII A and

VIII B). Second, MINX has been compared with ETOX,[5] number-by-number, for many isotopes (see Sec. VIII C). Finally, MINX libraries have been used to compute integral parameters. Results for six important fast reactor benchmarks are described in Sec. VIII D.

A second requirement of the MINX validation program was to prove that the IBM version of MINX developed at ORNL gave answers equivalent to the CDC-7600 version as run at LASL. Number-by-number comparisons with the 50-group library and integral comparisons are summarized in Sec. VIII E.

The libraries discussed in this section can be used as test problems for evaluating new versions of MINX.

A. The MINX 50-Group Library

LIB-IV[38] is a CCCC library of multigroup constants produced using MINX and NJOY[39] from ENDF/B-IV data and intended for (1) fast reactor core design, (2) CSEWG data testing, and (3) processing code comparison. The library contains cross sections, self-shielding factors, and delayed neutron constants (where available) for all the 90 materials of ENDF/B-IV plus the copper isotopes and lumped fission products from ENDF/B-III. The specifications for this library follow

1. Data source - ENDF/B-IV including revisions of June 1975 and ENDF/B-III for ^{63}Cu, ^{65}Cu, and lumped fission products.

2. Library format - CCCC-III,[23] ISOTXS, BRKOXS, and DLAYXS files (as appropriate). Structure of transmittal tape is given in Table III.

TABLE III

STRUCTURE OF LIB-IV TRANSMITTAL TAPES[a]

Tape	File	Contents	Number of Cards
	1	LINX	460
1	2	BINX	872
	3	CINX	857
	4	ISOTXS	192 273
2	5	BRKOXS	80 083
	6	DLAYXS	735
		Total	275 280

[a]Two seven track BCD tapes recorded at 800 BPI and blocked into records containing 50 card images of 80 columns each. The last block (record) in each file may be short.

3. Nuclides - 101 nuclides at zero Kelvin and infinite dilution plus three additional temperatures (300, 900, and 2100 K) and up to six additional values of σ_o as detailed in Table IV. The nine fission product files are named as follows: "N" means non-saturating, "S" means slowly saturating, and "R" means rapidly saturating. Delayed neutron yields and spectra are provided for seven isotopes: ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{129}Pu, ^{240}Pu, and ^{241}Pu.

4. Group structure - 50 groups including a thermal dump group (see Table V). This structure was tailored for fast reactors; it is a subset of the 240-group structure, and the commonly used 26-group half-lethargy structure is a subset of it.

5. Weight function - Thermal + 1/E + fission. The thermal portion is Maxwellian with a temperature of 0.025 eV which joins 1/E at 0.10 eV. The fission spectrum has a temperature of 1.4 MeV and joins 1/E at 820.8 keV (lower bound of group 6).

6. Legendre expansion - P_0 through P_3 matrices provided when data permits.

7. Tolerances - Resonance reconstruction 0.5%, linearization 0.2%, Doppler thinning 0.2%, and adaptive integration 0.1% (except ^{238}U, ^{103}Rh, and ^{133}Cs used a reconstruction tolerance of 1.0%).

Test results for this library are given below. Transmittal tapes are available from the National Neutron Cross Section Center (NNCSC) at Brookhaven National Laboratory.

B. The DCTR/DRRD 171 Group Library

The MINX program has been used in conjunction with the AMPX[25] system to produce a 171-group neutron library from ENDF/B-IV appropriate to design analysis problems for the Division of Controlled Thermonuclear Research and the Division of Reactor Research and Development of the Energy Research and Development Administration. This library[40] and its LMFBR 126-group subset[41] have been specified (as in Sec. VIII A) and fully documented elsewhere.[40,41] Significant testing[40,45] has already taken place and is continuing. Both of these libraries (and associated retrieval programs) are available upon request from the Radiation Shielding Information Center at Oak Ridge. It should also be noted that associated pointwise libraries are available in any of the aforementioned packages (Sec. VIII A and VIII B).

C. Comparisons Between MINX and ETOX

Direct comparisons between multigroup constants produced by ETOX[5] and MINX/CINX were made using a code which compared every number in two 22-isotope

TABLE IV

LIB-IV MATERIALS

I	MATERIAL	ENDF/B MAT NO.	MINX TIMING (SEC)	SIGO VALUES (BARNS)
1	H-1	1269	133	1000,100,10,1,.1,.01
2	H-2	1120	95	1000,100,10,1,.1,.01
3	H-3	1169	165	1000,100,10,1,.1,.01
4	HE-3	1146	102	10000,1000,100,10,1,.1
5	HE-4	1270	118	10000,1000,100,10,1,.1
6	LI-6	1271	157	1000,100,10,1,.1,.01
7	LI-7	1272	159	1000,100,10,1,.1,.01
8	BE-9	1289	516	1000,100,10,1,.1,.01
9	B-10	1273	428	1000,100,10,1
10	B-11	1160	182	100000,10000,1000,100,10,1
11	C-12	1274	156	1000,100,10,1,.1
12	N-14	1275	593	1000,100,10,1,.1,.01
13	O-16	1276	590	1000,100,10,1,.1
14	F	1277	384	10000,1000,100,10,1,.1
15	NA-23	1156	667	1000,100,10,1,.1
16	MG	1280	584	10000,1000,100,10,1,.1
17	AL-27	1193	631	100000,10000,1000,100,10,1
18	SI	1194	546	10000,1000,100,10,1,.1
19	CL	1149	438	10000,1000,100,10,1,.1
20	K	1150	368	10000,1000,100,10,1,.1
21	CA	1195	542	10000,1000,100,10,1,.1
22	TI	1286	218	100000,10000,1000,100,10,1
23	V	1196	344	100000,10000,1000,100,10,1
24	CR	1191	1641	1000,100,10,1,.1
25	MN-55	1197	705	100000,10000,1000,100,10,1
26	FE	1192	1075	1000,100,10,1,.1
27	CO-59	1199	910	10000,1000,100,10,1,.1
28	NI	1190	1251	1000,100,10,1,.1
29	CU	1295	707	100000,10000,1000,100,10,1
30	CU-63	1085	451	100000,10000,1000,100,10,1
31	CU-65	1086	365	100000,10000,1000,100,10,1
32	KR-78	1181	162	10000,1000,100,10,1,.1
33	KR-80	1182	178	10000,1000,100,10,1,.1
34	KR-82	1183	176	10000,1000,100,10,1,.1
35	KR-83	1184	192	10000,1000,100,10,1,.1
36	KR-84	1185	217	10000,1000,100,10,1,.1
37	KR-86	1186	163	10000,1000,100,10,1,.1
38	ZIRC-2	1284	1273	10000,1000,100,10,1,.1
39	NB-93	1189	2975	100000,10000,1000,100,10,1
40	MO	1287	532	100000,10000,1000,100,10,1
41	TC-99	1137	325	100000,10000,1000,100,10,1
42	RH-103	1125	2403	100000,10000,1000,100,10,1
43	AG-107	1138	698	100000,10000,1000,100,10,1
44	AG-109	1139	793	100000,10000,1000,100,10,1
45	CD	1281	839	10000,1000,100,10,1,.1
46	CD-113	1282	605	10000,1000,100,10,1,.1
47	XE-124	1170	177	10000,1000,100,10,1,.1

48	XE-126	1171	146	10000,1000,100,10,1,.1
49	XE-127	1172	307	10000,1000,100,10,1,.1
50	XE-128	1173	1165	10000,1000,100,10,1,.1
51	XE-130	1174	290	10000,1000,100,10,1,.1
52	XE-131	1175	751	10000,1000,100,10,1,.1
53	XE-132	1176	215	10000,1000,100,10,1,.1
54	XE-134	1177	143	10000,1000,100,10,1,.1
55	XE-135	1294	154	100000,10000,1000,100,10,1
56	XE-136	1178	128	100000,10000,1000,100,10,1
57	CS-133	1141	1472	100000,10000,1000,100,10,1
58	SM-149	1027	464	100000,10000,1000,100,10,1
59	EU-151	1290	900	100000,10000,1000,100,10,1
60	EU-152	1292	713	100000,10000,1000,100,10,1
61	EU-153	1291	785	100000,10000,1000,100,10,1
62	EU-154	1293	585	100000,10000,1000,100,10,1
63	GD	1030	378	100000,10000,1000,100,10,1
64	DY-164	1031	213	100000,10000,1000,100,10,1
65	LU-175	1032	354	100000,10000,1000,100,10,1
66	LU-176	1033	389	100000,10000,1000,100,10,1
67	TA-181	1285	1092	10000,1000,100,10,1,.1
68	TA-182	1127	252	10000,1000,100,10,1,.1
69	W-182	1128	2023	100000,10000,1000,100,10,1
70	W-183	1129	1353	100000,10000,1000,100,10,1
71	W-184	1130	1352	100000,10000,1000,100,10,1
72	W-186	1131	1489	100000,10000,1000,100,10,1
73	RE-185	1083	470	100000,10000,1000,100,10,1
74	RE-187	1084	418	100000,10000,1000,100,10,1
75	AU-197	1283	1685	100000,10000,1000,100,10,1
76	PB	1288	641	10000,1000,100,10,1,.1
77	TH-232	1296	3850	100000,10000,1000,100,10,1
78	PA-233	1297	462	100000,10000,1000,100,10,1
79	U-233	1260	531	10000,1000,100,10,1,.1
80	U-234	1043	672	100000,10000,1000,100,10,1
81	U-235	1261	2832	10000,1000,100,10,1,.1
82	U-236	1163	780	100000,10000,1000,100,10,1
83	U-238	1262	6454	10000,1000,100,10,1,.1
84	NP-237	1263	2085	100000,10000,1000,100,10,1
85	PU-238	1050	1043	100000,10000,1000,100,10,1
86	PU-239	1264	3505	10000,1000,100,10,1
87	PU-240	1265	6113	100000,10000,1000,100,10,1
88	PU-241	1266	544	100000,10000,1000,100,10,1
89	PU-242	1161	664	100000,10000,1000,100,10,1
90	AM-241	1056	540	100000,10000,1000,100,10,1
91	AM-243	1057	231	100000,10000,1000,100,10,1
92	CM-244	1162	1057	100000,10000,1000,100,10,1
93	FP235N	1067	83	10000,1000,100,10,1,.1
94	FP235S	1066	98	10000,1000,100,10,1,.1
95	FP235R	1042	93	10000,1000,100,10,1,.1
96	FP235N	1069	84	10000,1000,100,10,1,.1
97	FP235S	1068	93	10000,1000,100,10,1,.1
98	FP235R	1045	95	10000,1000,100,10,1,.1
99	FF239N	1071	85	10000,1000,100,10,1,.1
100	FP239S	1070	94	10000,1000,100,10,1,.1
101	FP239R	1052	91	10000,1000,100,10,1,.1
		TOTAL	79435	

TABLE V

LIB-IV GROUP STRUCTURE

GROUP	ENERGY RANGE (EV)		LETHARGY
01	1.5000E+07	1.0000E+07	0.692
02	1.0000E+07	6.0653E+06	0.5
03	6.0653E+06	3.6788E+06	0.5
04	3.6788E+06	2.2313E+06	0.5
05	2.2313E+06	1.3534E+06	0.5
06	1.3534E+06	8.2085E+05	0.5
07	8.2085E+05	4.9787E+05	0.5
08	4.9787E+05	3.8774E+05	0.25
09	3.8774E+05	3.0197E+05	0.25
10	3.0197E+05	2.3518E+05	0.25
11	2.3518E+05	1.8316E+05	0.25
12	1.8316E+05	1.4264E+05	0.25
13	1.4264E+05	1.1109E+05	0.25
14	1.1109E+05	8.6517E+04	0.25
15	8.6517E+04	6.7379E+04	0.25
16	6.7379E+04	5.2475E+04	0.25
17	5.2475E+04	4.0868E+04	0.25
18	4.0868E+04	3.1828E+04	0.25
19	3.1828E+04	2.4788E+04	0.25
20	2.4788E+04	1.9305E+04	0.25
21	1.9305E+04	1.5034E+04	0.25
22	1.5034E+04	1.1709E+04	0.25
23	1.1709E+04	9.1188E+03	0.25
24	9.1188E+03	7.1017E+03	0.25
25	7.1017E+03	5.5308E+03	0.25
26	5.5308E+03	4.3074E+03	0.25
27	4.3074E+03	3.3546E+03	0.25
28	3.3546E+03	2.6126E+03	0.25
29	2.6126E+03	2.0347E+03	0.25
30	2.0347E+03	1.5846E+03	0.25
31	1.5846E+03	1.2341E+03	0.25
32	1.2341E+03	9.6112E+02	0.25
33	9.6112E+02	7.4852E+02	0.25
34	7.4852E+02	5.8295E+02	0.25
35	5.8295E+02	4.5400E+02	0.25
36	4.5400E+02	3.5358E+02	0.25
37	3.5358E+02	2.7536E+02	0.25
38	2.7536E+02	1.6702E+02	0.5
39	1.6702E+02	1.0130E+02	0.5
40	1.0130E+02	6.1442E+01	0.5
41	6.1442E+01	3.7267E+01	0.5
42	3.7267E+01	2.2603E+01	0.5
43	2.2603E+01	1.3710E+01	0.5
44	1.3710E+01	8.3153E+00	0.5
45	8.3153E+00	5.0435E+00	0.5
46	5.0435E+00	3.0590E+00	0.5
47	3.0590E+00	1.8554E+00	0.5
48	1.8554E+00	1.1254E+00	0.5
49	1.1254E+00	6.8256E-01	0.5
50	6.8256E-01	1.0000E-05	11.13

libraries. The differences were mostly well within the MINX tolerances. Most of the larger differences were explained by the following problems.

1. The ETOX and MINX fission spectrum weighting function did not cut off at the same energy.

2. In the resonance regions, ETOX arbitrarily resets f-factors greater than one back to one.

3. ETOX does not correctly combine f-factor contributions in a group which contains the boundary between two resonance regions.

4. ETOX has errors in the treatment of discrete inelastic scattering and tabulated energy spectra from File 5.

5. ETOX does not weight $\bar{\nu}$, $\bar{\mu}$, and $\bar{\xi}$ with the fission or scattering reaction rate.

6. ETOX does not include (n,3n) or other high-threshold scattering reactions in its transfer matrix or inelastic cross section. All these problems taken together cause a difference in k_{eff} of less than 0.2% for a large Pu-fueled critical assembly.

D. CSEWG Critical Benchmarks

The 50-group library has been used in the calculation of six CSEWG benchmark critical assemblies to provide a comparison with results from other laboratories or other code systems and to give an indication of how the library will perform in reactor design calculations.

The MINX 50-group library was first converted to 1DX[42] format using an option of CINX. Values for k_{eff} and the reaction rate ratios were then computed directly with 1DX for the large assemblies. The smaller assemblies were computed with DTF-IV[43] using self-shielded macroscopic cross section from 1DX. The results are summarized in Tables VI and VII. These results are in general agreement with those obtained by other methods[44,45] and with libraries containing larger numbers of groups.

E. Comparison of CDC and IBM Version of MINX

In an effort to demonstrate that the IBM version of MINX produces the same multigroup constants (within acceptable precision tolerance due to the difference in word size on the two machines) as the base CDC code, several nuclides were selected from the LASL 50-group cross-section library for a detailed number-by-number comparison. The purpose of this section is to summarize these comparisons for Fe, O-16, U-235, U-238, and Pu-241 cross sections. It is hoped that

TABLE VI

CSEWG BENCHMARK EIGENVALUES

Benchmark	Codes Used	Uncorrected Keff	Heterogeneity Correction	$P_0 \rightarrow P_\infty$ Correction	Diff$\rightarrow S_8$ Correction	$S_{16} \rightarrow S_\infty$ Correction	Corrected Keff
Pu Fueled*							
JEZEBEL	1DX-DTF	1.00089		-0.0032		-0.0021	0.99559
VERA-11A	1DX-DTF	0.99235				-0.002	0.99035
ZPR-6-7	1DX	0.97085	0.0166		0.0018		0.98925
U Fueled*							
GODIVA	1DX-DTF	1.01184		-0.003		-0.0017	1.00714
ZPR-3-11	1DX-DTF	1.01515					1.01515
ZPR-6-6A	1DX	0.98323	0.0073		0.0013		0.99183

*Arranged in order of spectrum hardness.

TABLE VII

CENTRAL SPECTRAL INDICES (CALCULATED-TO-EXPERIMENTAL)

Ratio W.R.T U-235(n,f)	Pu-Fueled*			U-Fueled*		
	JEZEBEL	VERA-11A	ZPR-6-7	GODIVA	ZPR-3-11	ZPR-6-6A
Pu-240(n,f)		1.0850			1.0540	
Pu-239(n,f)	0.9363	1.0836	0.9625	0.9728	0.9843	
U-238(n,f)	0.9485	1.1531	0.9377	1.0861	1.0563	0.9452
U-238(n,γ)			1.0534	0.9925	0.9691	1.0309
Np-237(n,f)	0.9448	1.1758			1.0506	
U-236(n,f)					0.7851	
U-234(n,f)				0.9762	1.0405	
U-233(n,f)	0.9287	0.9993		0.9241	0.9989	
Th-232(n,f)				1.0758		
Au(n,γ)				0.8491		

*Arranged in order of spectrum hardness.

the aforementioned nuclides are representative of ENDF/B-IV light, medium, and heavy materials and that they illustrate general processing trends with respect to the algorithms invoked.

The following comments and examples attempt to say something meaningful about LASL and ORNL results at various checkpoints throughout the calculation.

1. Pointwise Reconstruction from Resonance Parameters - There are minor differences in the number of points generated and rejected by the RESEND overlay. The ORNL version usually tends to generate more points. Table VIII contains the infinitely dilute 0 K pointwise results for Fe, U-235, U-238, and Pu-241.
2. Doppler Broadening and Linearization - The linearization process creates a different number of points when using the IBM version (see Table IX).
3. Generation of Self-Shielded Cross Sections in the Unresolved Energy Range - No significant differences observed.
4. Group Averaging of the Smooth Cross Sections - The infinitely dilute and shielded cross-section values generally agree for the five digits of significance edited by MINX. Discrepancies were found and the percent

TABLE VIII

COMPARISON OF LASL AND ORNL RESEND OVERLAYS FOR U-238, U-235, Pu-241, and Fe

LAB	ENDF/B MAT	Reconstruction Tolerance	Temperature	Number of Points Resonance Range	Number of Points Rejected by Truncation Algorithm
LASL	1261	0.005	0 K	6042	0
LASL	1262	0.01	0 K	49943	14609
LASL	1266	0.005	0 K	1908	0
LASL	1192	0.005	0 K	4176	853
ORNL	1261	0.005	0 K	6039	0
ORNL	1262	0.01	0 K	50096	15081
ORNL	1266	0.005	0 K	1915	0
ORNL	1192	0.005	0 K	4215	890

TABLE IX

COMPARISON OF LASL AND ORNL LINEARIZATION RESULTS FOR Fe(MAT 1192) AND O-16(MAT 1276)

LAB	ENDF/B MAT	MT	Interpolation Table Before*	NP After Linearization
LASL	1192	4	2 2 534 4	2051
ORNL	1192	4	2 2 534 4	1985
LASL	1192	51	2 2 465 4	2009
ORNL	1192	51	2 2 465 4	1944
LASL	1276	102	3 5	50
ORNL	1276	102	3 5	117

*As in ENDF/B format (Ref. 1).

error was less than the integration tolerance for those nuclides tested. Needless to say, small cross sections and resonance energy range cross sections represented the largest sources of discrepancies. Examples are given in Table X.

5. Elastic Scattering Transfer Matrix Calculation - The P_0 terms generally agree with disagreement seen in the higher order terms. The disagreement in the P_n terms tend to increase with increasing Legendre order with the worst disagreement in the highest order term. For all Legendre components of the group-to-group elastic scattering cross sections, the values differ most for very small contributions with the worst discrepancy seen in the within-group term. Examples are given in Table XI.
6. Discrete Inelastic and Continuum Transfer Matrix Calculation - Comparisons of these cross sections indicate the same type of behavior as the elastic scattering group-to-group cross sections.

In summary, the dominant impression gained from the testing experience is that given the same pointwise cross-section file, the multigroup averaging calculation is equivalent on the two machines with the only exception being the high order group-to-group transfer cross sections. Discrepancies in the high order components are most dramatic where the absolute value is very small. A selected group of core and shield analysis problems have been studied using MINX/IBM cross sections and these differences have had no impact to date.

TABLE X

COMPARISON OF LASL AND ORNL MULTIGROUP AVERAGED RESULTS FOR U-235(MAT 1261) AND O-16(MAT 1276)*

50-Group Number	Nuclide	Reaction	LASL	ORNL	% Error
38	U-235	MT=1	43.965	43.965	0
39	U-235	MT=1	47.163	47.162	0.002
40	U-235	MT=1	48.312	48.315	0.006
41	U-235	MT=1	79.756	79.760	0.005
42	U-235	MT=1	92.362	92.369	0.008
43	U-235	MT=1	95.490	95.484	0.006
44	U-235	MT=1	144.66	144.66	0.
1	O-16	MT=1	1.4986	1.4986	0.
2	O-16	MT=1	1.1194	1.1194	0.
3	O-16	MT=1	1.8336	1.8336	0.
4	O-16	MT=1	1.5681	1.5681	0.
.					
.					
.					
49	O-16	MT=1	3.7481	3.7481	0.
50	O-16	MT=1	3.7483	3.7483	0.

*The cross sections are infinitely dilute at 0 K.

TABLE XI

COMPARISON OF LASL AND ORNL ELASTIC SCATTERING
GROUP-TO-GROUP TRANSFER CROSS SECTIONS

$\sigma(g \rightarrow g')$	Nuclide	P_0 LASL	P_0 ORNL	% Error	P_2 LASL	P_2 ORNL	% Error
$\sigma(50 \rightarrow 50)$	U-235	1.5054E+1	1.5054E+1	0.	5.5448E-5	-2.3849E-4	330.
$\sigma(49 \rightarrow 49)$	U-235	1.2788E+1	1.2788E+1	0.	3.7595E-4	8.6196E-5	73.6
$\sigma(49 \rightarrow 50)$	U-235	0.22970	0.22970	0.	-2.7800E-4	-2.8894E-4	3.94
$\sigma(48 \rightarrow 48)$	U-235	1.2401E+1	1.2400E+1	0.008	2.3293E-4	5.6086E-5	75.9
$\sigma(48 \rightarrow 49)$	U-235	0.22180	0.22182	0.009	-1.8644E-4	-1.8862E-4	1.2
$\sigma(47 \rightarrow 47)$	U-235	1.1579E+1	1.1578E+1	0.009	3.0221E-4	1.0820E-4	64.2
$\sigma(47 \rightarrow 48)$	U-235	0.20668	0.20669	0.005	-2.5881E-4	-2.6420E-4	2.1
$\sigma(14 \rightarrow 14)$	O-16	1.7299	1.7299	0.	-1.2625E-3	-1.2741E-3	0.9
$\sigma(14 \rightarrow 15)$	O-16	1.8453	1.8453	0.	1.3791E-3	1.3911E-3	0.9
$\sigma(14 \rightarrow 16)$	O-16	1.9362E-4	1.9362E-4	0.	-1.8582E-4	-1.8569E-4	0.07
$\sigma(3 \rightarrow 3)$	O-16	1.2592	1.2591	0.008	0.28829	0.28823	0.02
$\sigma(3 \rightarrow 4)$	O-16	0.51483	0.51481	0.004	-9.4981E-3	-9.4949E-3	0.03
$\sigma(2 \rightarrow 2)$	O-16	0.59552	0.59550	0.003	0.14307	0.14305	0.01
$\sigma(2 \rightarrow 3)$	O-16	0.31489	0.31489	0.	2.8225E-2	2.8226E-2	0.004
$\sigma(1 \rightarrow 1)$	O-16	0.66384	0.66378	0.009	0.26490	0.26486	0.02
$\sigma(1 \rightarrow 2)$	O-16	0.33732	0.33731	0.003	4.9628E-3	4.9666E-3	0.08

3. Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{\ell=0}^{NLS} \sigma_{n,f}^{\ell}(E) \quad , \tag{A-5}$$

where

$$\sigma_{n,f}^{\ell}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{fr}}{(E-E_r')^2 + \frac{1}{4}\Gamma_4^2} \quad , \tag{A-6}$$

where

$$g_J = \frac{2J+1}{2(2I+1)} \quad . \tag{A-7}$$

I is the spin of the target nucleus and J is the spin of the compound nucleus for the resonance state. *I = SPI, as given in File 2 for data for each isotope.* The summation on ℓ extends over all ρ-states described. There will be NLS terms in the summation. *NLS is given in File 2 for each isotope.* The summation on J extends over all possible J-states for a particular ℓ-state, NR_J is the number of resonances for a given pair of ℓ and J values.

$$NRS = \sum_{J} NR_J \quad .$$

$\Gamma_{nr}(|E_r|) \equiv GN_r$ is the neutron width, for the r^{th} resonance for a particular value of ℓ, evaluated at the resonance energy E_r. For bound levels, the absolute value $|E_r|$ is used.

$$\Gamma_{nr} = \frac{P_\ell(E)\ \Gamma_{nr}(|E_r|)}{P_\ell(|E_r|)} \quad , \tag{A-8}$$

$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr}$ is the total width.

The following quantities are given in File 2 for each resonance

E_r = ER, the resonance energy.

J = AJ, the spin of the resonance state.

$\Gamma_{nr}(|E_r|)$ = GN, the neutron width.

$\Gamma_{\gamma r}$ = GG, the radiation width.

Γ_{fr} = GF, the fission width.

$$E'_r = E_r + \frac{S_\ell(|E_r|) - S_\ell(E)}{2P_\ell(|E_r|)} \Gamma_{nr}(|E_r|) , \tag{A-9}$$

and

$$k = 2.196771 \frac{AWRI}{AWRI + 1.0} 10^{-3} \sqrt{E} , \tag{A-10}$$

where k is the neutron wave number and AWRI is the ratio of the mass of the particular isotope to that of the neutron. *AWRI given in File 2 data for each isotope.* E is incident neutron energy (laboratory system); S_ℓ is the shift factor,

$$S_0 = 0 ,$$

$$S_1 = -\frac{1}{1 + \rho^2} , \text{ and}$$

$$S_2 = -\frac{18 + 3\rho^2}{9 + 3\rho^2 + \rho^4} . \tag{A-11}$$

P_ℓ is the penetration factor,

$$P_0 = \rho ,$$

$$P_1 = \frac{\rho^3}{1 + \rho^2} , \text{ and}$$

$$P_2 = \frac{\rho^5}{9 + 3\rho^2 + \rho^4} , \tag{A-12}$$

where $\rho = ka$ and "a" is the channel radius (in units of 10^{-12}cm) and is defined as

$$a = [1.23(AWRI)^{1/3} + 0.8] \times 10^{-1}, \tag{A-13}$$

and ϕ_ℓ is the phase shift,

$$\phi_0 = \hat{\rho} \ ,$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho} \ , \text{ and}$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\frac{3\hat{\rho}}{3 - \hat{\rho}^2} \ , \tag{A-14}$$

where $\hat{\rho} = k\hat{a}$ and $\hat{a}$ is the effective scattering radius. *$\hat{a} = AP$, as given in File 2 data.*

B. Multilevel Breit-Wigner Formula: LRU=1 LRF=2. (This section is taken directly from Ref. 28 and is discussed with reference to the formulas presented in the ENDF Formats and Procedures Manual.[1])

$$\sigma_{nn}(E) = \sum_{\ell=0}^{NLS} \sigma_{nn}^{\ell}(E) \ , \tag{A-15}$$

$$\sigma_{nn}^{\ell}(E) + \frac{\pi}{k^2} \sum_{J}^{NR_j} g_J \left|1 - U_{nn}^{J}(E)\right|^2 \ , \text{ and} \tag{A-16}$$

$$U_{nn}^{J}(E) = \exp(2i\phi_\ell) - \sum_{r=1}^{NR_J} \frac{i\Gamma_{nr}}{E_r' - E - i\Gamma_r/c}, \tag{A-17}$$

where the symbols are standard to the Formats and Procedures Manual. Equation (A-17) may be written

$$U_{nn}^{J}(E) = \cos(2\phi_\ell) + i \sin(2\phi_\ell) - \sum_{r=1}^{NR_j} \frac{i\Gamma_{nr}}{E_r' - E - i\,\Gamma_r/2} \ . \tag{A-18}$$

Substituting Eq. (A-18) in Eq. (A-16), making the substitution

$$X_r = 2(E - E'_r)/\Gamma_r \quad , \tag{A-19}$$

and noting the modulus $|a + ib|^2 = a^2 + b^2$ we obtain the working equation

$$\sigma^{\ell}_{nn}(E) = \frac{\pi}{k^2} \sum_J g_J \left\{ \left(\left[1 - \cos 2\phi_\ell \right] - \sum_{r=1}^{NR_J} \frac{2\Gamma_{nr}/\Gamma_r}{1 + X_r^2} \right) + \left(\sin 2\phi\ell + \sum_{r=1}^{NR_J} \frac{2X_r \Gamma_{nr}/\Gamma_r}{1 + X_r^2} \right)^2 \right\} \quad . \tag{A-20}$$

The consistent equations for capture and fission are

$$\sigma_{nr} = \frac{2\pi}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \frac{2\Gamma_{nr}/\Gamma_r(\Gamma_{\gamma r}/\Gamma_r)}{1 + X_r^2} \tag{A-21}$$

$$\sigma_{nf} = \frac{2\pi}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \frac{2\Gamma_{nr}/\Gamma_r(\Gamma_{fr}/\Gamma_r)}{1 + X_r^2} \quad . \tag{A-22}$$

The elastic scattering equation used in RESEND, taken from the Formats and Procedures Manual is

$$\sigma_{nn}(E) = (2\ell + 1)\frac{4\pi}{k^2}\sin^2\phi_\ell$$

$$+\frac{\pi}{k^2}\sum_J\sum_{r=1}^{NR_J}\frac{\Gamma_{nr}^2\cos2\theta_\ell - 2\Gamma_{nr}(\Gamma_{\gamma r}+\Gamma_{fr})\sin^2\theta_\ell + 2(E-E_r')\Gamma_{nr}\sin2\theta_\ell}{(E-E_r')^2+(\Gamma_r/2)^2}$$

$$+\frac{\pi}{k^2}\sum_J\sum_{r=2}^{NR_J}\sum_{s=1}^{r-1}\frac{2\Gamma_{nr}\Gamma_{ns}[(E-E_r')(E-E_s')+\Gamma_r\Gamma_s/4]}{[(E-E_r')^2+(\Gamma_r/2)^2][(E-E_s')^2+(\Gamma_s/2)^2]}\cdot \qquad \text{(A-23)}$$

The general non-interference terms in Eq. (A-23) may be rewritten as

$$\frac{4(\Gamma_{nr}/\Gamma_r)\{(\Gamma_{nr}/\Gamma_r)[\cos2\phi_\ell + 2\sin^2\phi_\ell] - 2\sin^2\phi_\ell + X_r\sin2\phi_\ell\}}{1+X_r^2} \qquad \text{(A-24)}$$

by substituting Eq. (A-19) and noting that $\Gamma_r = \Gamma_{nr} + \Gamma_{\gamma r} + \Gamma_{fr}$.

Eq. (A-24) may be further reduced by use of the trigonometric identity

$$1 - \cos2\phi_\ell = 2\sin^2\phi_\ell \qquad \text{(A-25)}$$

to yield

$$\frac{4\Gamma_{nr}/\Gamma_r(\Gamma_{nr}/\Gamma_r - 2\sin^2\phi_\ell + X_r\sin2\phi_\ell)}{1+X_r^2}\cdot \qquad \text{(A-26)}$$

Now, if Eq. (A-23) is squared and the non-interference terms are collected,

$$\frac{-2(1 - \cos 2\phi_\ell)(2\Gamma_{nr}/\Gamma_r)}{1 + X_r^2} + \frac{(2\Gamma_{nr}/\Gamma_r)^2}{(1 + X_r^2)^2}$$

$$+ \frac{2\sin^2\phi_\ell(2X_r\Gamma_{nr}/\Gamma_r)}{1 + X_r^2} + \frac{(2X_r\Gamma_{nr}/\Gamma_r)^2}{(1 + X_r^2)^2} \quad . \tag{A-27}$$

Combining terms gives

$$\frac{4\Gamma_{nr}/\Gamma_r(\Gamma_{nr}/\Gamma_r - (1 - \cos 2\phi_\ell) + X_r \sin 2\phi_\ell)}{1 + X_r^2} \quad , \tag{A-28}$$

which is identical to Eq. (A-26) by virtue of the trigonometric identity Eq. (A-25).

In a similar fashion it can be shown that the interference terms are also identical in Eqs. (A-20) and (A-23).

The first term in Eq. (A-23) is equivalent to the potential scattering terms of Eq. (A-22), i.e.,

$$\begin{aligned}
&\frac{\pi}{k^2} \sum_J g_J[1 - \cos 2\phi_\ell]^2 + g_J[\sin 2\phi_\ell]^2 \\
&= \frac{\pi}{k^2} \sum_J g_J[1 - 2\cos 2\phi_\ell + \cos^2(2\phi_\ell) + \sin^2(2\phi_\ell)] \\
&= \frac{4\pi}{k^2} \sin^2\phi_\ell \sum_J g_J \\
&= \frac{4\pi}{k^2}(2\ell + 1)\sin^2\phi_\ell \quad .
\end{aligned} \tag{A-29}$$

As pointed out by C. Lubitz in Ref. 28, the sum on J in the identity

$$\sum_J g_J = 2\ell + 1 \tag{A-30}$$

used in Eq. (A-29) goes over all allowed J values for a given target spin I and angular momentum ℓ. Thus the potential terms must be summed over all J values from

$$|(|I - 1/2|-\ell)| \text{ to } |I - 1/2| + \ell \text{ for channel spin } I - 1/2, \quad \text{(A-31)}$$

and from

$$|I + 1/2 - \ell| \text{ to } I + 1/2 + \ell \text{ for channel spin } I + 1/2. \quad \text{(A-32)}$$

The dramatic savings in computational time, of course, arises from the calculation of $\sigma_{elastic}$ (E) using Eq. (A-20) which requires a sum of n resonance terms rather than Eq. (A-23) which requires a sum of n^2 terms.

Modest program modifications were required to implement this scheme. In RESEND the basic File 2 data is read in subroutine RDFIL2, but the resonance parameter data for each formalism is read by a separate routine. The subroutine that reads the MLBW parameters was modified to calculate the allowable J state sequences [Eqs. (17) and (18)] and store the index of the J state rather than the statistical weight factor g_J for each resonance. A separate array GJ was set up to store the statistical weight factors.

A maximum of 10 J values are allowed in the current version. Error stop 298 flags a case requiring more than 10 J values for any particular ℓ sequence. In indexing the values of J for each resonance, error stop 297 flags a non-allowed J value, while error stop 299 flags the condition $\Sigma_J g_J \neq 2\ell + 1$. The use of the fictitious J value J = I which produces an average g factor of 1/2 is then prohibited. The complex-amplitude form of MLBW relies on the sum of J being carried out correctly, in order to produce the correct potential scattering cross section.

The MLBW calculation of cross sections as a function of energy occurs in the CSMLBW subroutine which was modified to calculate Eqs. (A-20) through (A-22).

An array SIGJ was used to store the separate J-dependent elastic scattering terms in the resonance loop. A final sum is then made over all J states before looping to the new value of ℓ.

C. Reich-Moore Formulae. MINX does not process Reich-Moore formula data since no such data appear in the files and such data may be converted equivalently to Adler-Adler format. A detailed derivation of these formulas is to be found in a paper by Reich and Moore.[47] Neutron cross sections with an exit channel c are given by*

$$\sigma_{nc} = \pi\lambda_n^2 \sum_J g_J \left|\delta_{nc} - U^J_{nc}\right|^2 \quad , \tag{A-33}$$

where λ_n is calculated in the center-of-mass system; and

$$\frac{1}{\lambda_n} = k_n = 2.196771\left(\frac{\text{AWRI}}{\text{AWRI} + 1.0}\right) \times 10^{-3} \sqrt{E(eV)} \quad , \tag{A-34}$$

where AWRI is the mass of the target nucleus in units of neutron mass. The statistical factor

$$g_J = \frac{(2J + 1)}{2(2I + 1)} \quad , \tag{A-35}$$

where J is the spin of the compound nucleus resonance and I is the target nucleus spin.

In terms of the Reich-Moore approximation one may write

$$U^J_{nc} = e^{-e(\phi_n + \phi_c)} \left\{2[(I - K)^{-1}]_{nc} - \delta_{nc}\right\} \quad , \tag{A-36}$$

where

$$(I-K)_{cc'} = \delta_{cc'} - \frac{i}{2} \sum_\Gamma \frac{\Gamma^{1/2}_{\gamma c} \Gamma^{1/2}_{c'}}{E_\lambda - E - \frac{i}{2}\Gamma_{\lambda\gamma}} \quad , \tag{A-37}$$

*These formulas are to be used for the 0 K case (no Doppler broadening terms given).

where the summation in Eq. (A-37) is over the resonance levels λ; E_λ is the resonance energy; $\Gamma_{\lambda\gamma}$, the corresponding radiation widths; and $\Gamma_{\lambda c}$ and $\Gamma_{\lambda c'}$ are the widths for the λ-th level and channels c and c', respectively.

If we define

$$\rho_{nc} = \delta_{nc} - [(I - K)^{-1}]_{nc} = \delta_{nc} - \frac{m_{nc}}{\Delta} \quad ,$$

where $\Delta = |I-K|$ the detriment of the matrix I-K and m_{nc} is the co-factor of the element $(I-K)_{nc}$ of the matrix I-K, we obtain

$$\sigma_{nT} = \sum_J \sigma^J_{nT} = 2\pi \lambda^2_n \sum_J g_J \, \mathrm{Re}\left(1 - U^J_{mn}\right)$$

$$= 2\pi \lambda^2_n \sum_J \left\{ g_J(1-\cos 2\phi_n) + 2g_J \mathrm{Re}\left(e^{-2i\rho_n}\rho_{nn}\right)\right\} . \qquad \text{(A-38)}$$

$$\sigma_{nn} = \pi\lambda^2_n \sum_J g_J |1 - U^2_{nn}|^2 \, , \qquad \text{(A-39)}$$

$$\sigma_{nAbs} = \sigma_{nT} - \sigma_{nn} = 4\pi\lambda^2_n \sum_J g_J \left[\mathrm{Re}(\rho_{nn}) - |\rho_{nn}|^2\right] , \qquad \text{(A-40)}$$

$$\sigma_{nFiss} = 4\pi\lambda^2_n \sum_J g_J \left(\sum_c |\rho_{nc}|^2\right) \quad , \qquad \text{(A-41)}$$

$$\sigma_n = \sigma_{nAbs} - \sigma_{nFiss} \, . \qquad \text{(A-42)}$$

For s-wave neutrons $\phi_n = +k_n a$ where k_n has been defined by Eq. (A-34) and a is the channel radius. For p- and d-wave resonances, ϕ_n is defined by Eq. (A-14).

D. Adler-Adler Multilevel Resonance Parameters: LRU=1, LRF=2. The formulas for obtaining cross sections have been taken from Adler and Adler.[48,49] These are given for the total, radiative capture and fission cross sections (without Doppler broadening).

1. Total Cross Section

$$\sigma_T(E) = \frac{2C}{E}(1-\cos\omega)$$

$$+ \frac{C}{\sqrt{E}} \sum_{R=1}^{NRS} \frac{\nu_R^T\left[G_R^T \cos\omega + H_R^T \sin\omega\right] + \left(\mu_R^T - E\right)\left[H_R^T \cos\omega - G_R^T \sin\omega\right]}{\left(\mu_R^T - E\right)^2 + \left(\nu_R^T\right)^2}$$

$$+ \frac{C}{\sqrt{E}} (AT_1 + AT_2/E + AT_3/E^2 + AT_4/E^3 + BT_1 * E + BT_2 * E^2) \quad . \qquad \text{(A-43)}$$

2. Capture Cross Section

$$\sigma_{n,\gamma}(E) =$$

$$\frac{C}{\sqrt{E}} \sum_{R=1}^{NRS} \frac{\nu_R^\gamma \left[G_R \cos\omega + H_R \sin\omega\right] + \left(\mu_R^\gamma - E\right)\left[H_R^f \cos\omega - G_R \sin\omega\right]}{\left(\mu_R^\gamma - E\right)^2 + \left(\nu_R^f\right)^2}$$

$$+ \frac{C}{\sqrt{E}} (AC_1 + AC_2/E + AC_3/E^2 + AC_1/E^3 + BC_1 * E + BX_2 * E^2) \qquad \text{(A-44)}$$

3. Fission Cross Section

$$\sigma_{n,f}(E) =$$

$$\frac{C}{\sqrt{E}} \sum_{R=1}^{NRS} \frac{\nu_R^f \left[G_R^f \cos\omega + H_R^f \sin\omega\right] + \left(\mu_R^f - E\right) \left[H_R^f \cos\omega - G_R^f \cos\omega - G_R^f \sin\omega\right]}{\left(\mu_R^f - E\right)^2 + \left(\nu_R^f\right)^2}$$

$$+ \frac{C}{\sqrt{E}} \left(AF_1 + AF_2/E + AF_3/E^2 + AF_4/E^3 + BF_1 * E + BF_2 * E^2\right),$$

$$\omega = 2\, k\hat{a}, \qquad \text{(A-45)}$$

where k is the neutron wave number

$$k = 2.196771 \left(\frac{AWRI}{AWR + 1.0}\right) 10^{-3} \sqrt{E(eV)} ,$$

$\hat{a}$ = AP = effective scattering radius (in units of 10^{-12} cm), and

$$\frac{C}{E} = \pi\lambda^2 = \frac{\pi}{k^2} .$$

APPENDIX B

POINT CROSS-SECTION GENERATION

The major consideration[27] in generating tabular data files is the selection of a proper convergence or accuracy criterion. When reducing ENDF/B files into a linearized tabular form two problems are encountered:

(a) Conversion of cross-section data which are already in tabular form but may have a logarithmic or semilogarithmic functional dependence between the tabulated points into a linear tabulation (linearization). The linearized form is required for the kernel broadening procedure which is used subsequently.

(b) Processing of data given in parametric form (e.g., resonance range data) into tables with an energy grid selected in a manner to insure the fewest number of points for a desired accuracy.

Both of these problems can be considered as approximating a function f(E) defined for all E, by another $\overline{f}(E)$ such that: $\overline{f}(E_i) \equiv f(E_i)$ at the tabulated points E_i, and the deviation between an interpolated point f(E) and the true value f(E) is less than some user-specified value for all E between successive tabulated entries.

For inherently positive functions such as a cross section the convergence between tabulated points should be determined on the basis of the fractional difference, i.e., $|\overline{f}(E) - f(E)| < \varepsilon f(E)$, as opposed to the absolute difference $|\overline{f}(E) - f(E)| < \varepsilon$.

Criteria based on the fractional difference are consistent with uncertainties in the experimental data and result in a more uniform distribution of data points in low as well as high cross-section areas.

A numerical "interval halving" algorithm incorporated into the code RESEND[22] and compatible with the fractional difference criterion has been found well suited for the generation of tabular files in the resonance range as well as for the linearization of already tabular ENDF/B data files. This algorithm consists of the following steps:

(a) A set of initial energy "node points" is selected. For tabular data, nodes are located at the edges of nonlinear interpolation ranges. For resonance data, nodes are set at the peaks of resonances.

(b) The exact cross section f(E) is calculated at the node points and $\overline{f}(E)$ is set equal to f(E).

(c) The value of the approximate function $\overline{f}(E)$ at the mid-point between two nodes is obtained by linear interpolation and compared with the exact value f(E) at the same point. If the fractional difference at the mid-point is larger than the desired convergence criterion, the mid-point is defined to be a new node and the process repeated in the halved interval. When a difference smaller than the convergence criterion is reached, the interval is assumed to have converged and the process is repeated between the next set of nodes (Fig. B-1).

When generating tabular cross-section files from resonance parameter data, the convergence test is applied to each of the individual reaction types separately and not limited to the total cross section, since variations in

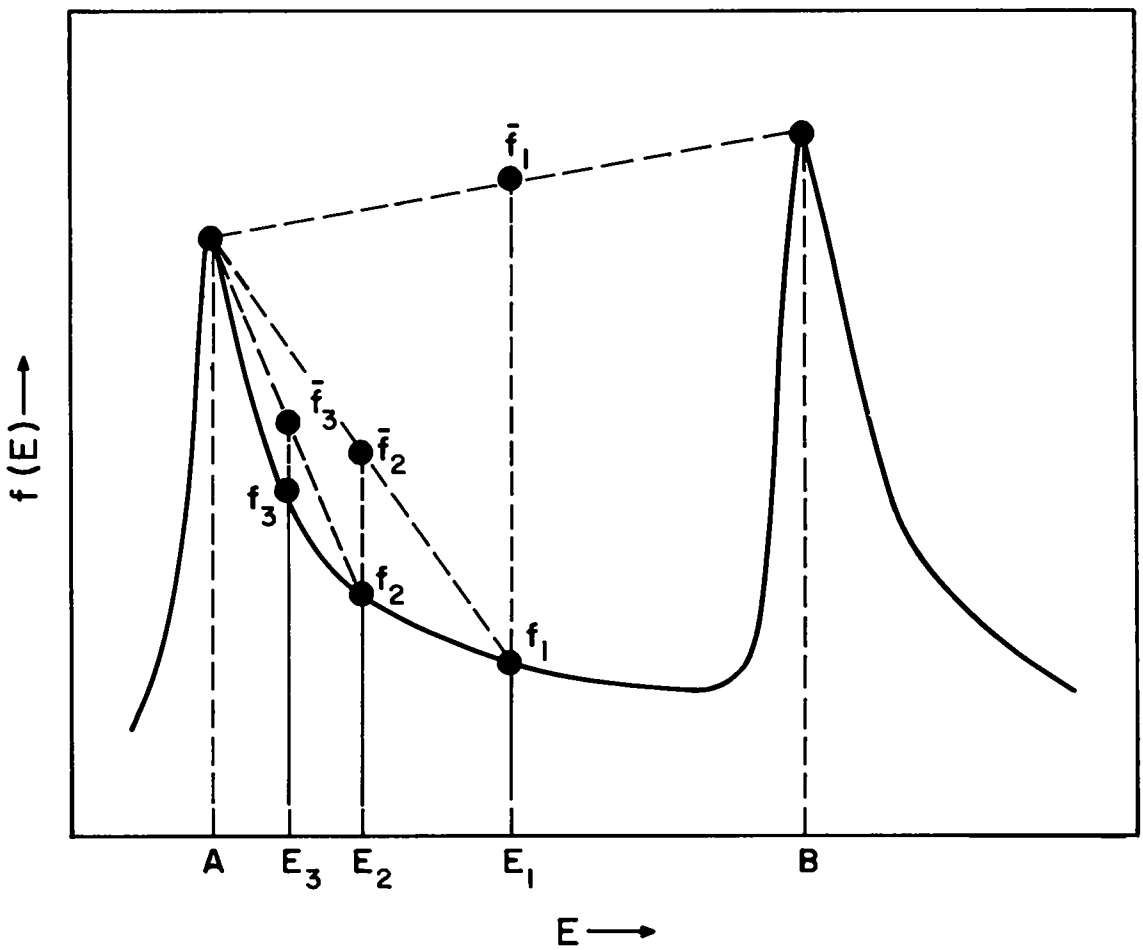

Fig. B-1. Generation of energy grid in program RESEND.

reaction types with a low cross section, (e.g., interference dips in elastic scattering) tend to be washed out when contributions from other, larger reactions are added on.

For the process of linearization of data tables, an algorithm based on the maximum in the absolute difference $|f(E) - \bar{f}(E)|$ has been developed and implemented (for the linearization of those interpolation laws permitted in ENDF/B). These are described in detail in Appendix C.

APPENDIX C

LINEARIZATION OF ENDF/B INTERPOLATION LAWS

ENDF/B data formats are selected to facilitate representation of nuclear physics information arising in the data evaluation process. Such "evaluation" formats include a variety of interpolation schemes. For rapid retrieval during Monte Carlo and processing code execution, it is desirable that no interpolation scheme more sophisticated than linear-linear be employed. In log-log interpolation, three logarithms and one exponentiation are required to interpolate one cross section. Moreover, piecewise linear representation of cross-section behavior allows for the introduction of a rapid, semi-analytic kernel broadening scheme used to consider temperature-dependent effects.

Consider a pair of successive points (e.g., energies) and associated dependent variables (e.g., cross sections) X1, Y1, and X2, Y2 along with one of the following five interpolation schemes

Scheme	Type	Formula	
1	Y constant and equal to the value at the lower end of the interval	$Y = Y1$	(C-1)
2	Y linear in X	$Y = Y1+(X-X1)(Y2-Y1)/(X2-X1)$	(C-2)
3	Y linear in ln X	$Y = Y1+\ln(X/X1)(Y2-Y1)/\ln(X2/X1)$	(C-3)
4	ln Y linear in X	$Y = Y1\{EXP[(X-X1)\ \ln(Y2/Y1)/(X2-X1)]\}$	(C-4)
5	ln Y linear in ln X	$Y = Y1\{EXP[\ln(X/X1)\ \ln(Y2/Y1)/\ln(X2/X1)]\}$.	(C-5)

Let ε_1 define an acceptable tolerance such that linear interpolation between X1 and X2 resulting in cross section YLIN at point X (bounded by X1 and X2) is equivalent to the cross section YM computed at point X using the correct interpolation scheme. That is,

$$\left|\frac{YLIN(X) - YM(X)}{YM(X)}\right| \leq \varepsilon_1. \qquad (C-6)$$

One proceeds by computing the point X, denoted by XM, located between X1 and X2 where the difference between YLIN and YM is a maximum, and then determines whether the relative difference lies with ε_1. If this condition is satisfied the next set of points (X2, Y2, and X3, Y3) is examined. Otherwise the point XM is added with the respective dependent variable YM and the process repeated (with X1, Y1, and XM, YM) until Eq. (C-6) is satisfied for all X bounded by X1 and XM. The process is then continued using XM, YM, and X2, Y2, and so on until the entire data set is spanned.

A. Determination of XM for Schemes 1 and 2. For constant and linear-linear variations it is unnecessary to add any points. However, the following equations apply for Eqs. (C-3) through (C-5). Note that subscript ones and twos have been interchanged for convenience. This obviously does not affect any of the results.

B. Determination of XM for Scheme 3.

$$Y = Y2+\ln(X/X2)(Y1-Y2)/\ln(X1/X2), \qquad (C-7)$$

$$Y = A+B\ln X, \qquad (C-8)$$

where

$$A = Y2 - (B)(\ln X2), \qquad (C-9)$$

$$B = (Y1-Y2)/\ln(X1/X2) \quad . \qquad (C-10)$$

Now, the linear-linear representation was given in Eq. (C-2) which is reformulated here as

$$Y = Y2+(C5)(X-X2), \qquad (C-11)$$

where

$$C5 = (Y1-Y2)/(X1-X2). \tag{C-12}$$

Consider the function

$$F(X) = A+B\ln X-[(Y2+(C5)(X-X2)].$$

F(X) represents the difference between the semilog representation [Eq. (C-3)] and a linear representation [Eq. (C-2)]. The point XM where F(X) has its maximum is found by differentiation and setting the resulting equation equal to zero.

$$F'(X) = \frac{B}{X} - C5 = 0. \tag{C-13}$$

Hence ,

$$XM = B/C5. \tag{C-14}$$

Since neither the linear-linear nor semilog formula has inflection points over the range X1 to X2, the point XM lying between X1 and X2 must represent a point of maximum difference. This is also clear since B&n(X) is always negative.

C. Determination of XM for Scheme 4. Consider Eq. (C-4) in the form

$$Y = [Y2 \exp(\{X-X2\}B)], \tag{C-15}$$

where

$$B = \ln(Y1/Y2)/(X1-X2). \tag{C-16}$$

Construct the functional difference

$$F(X) = Y2[\exp(B\{X-X2\})] - (Y2+C5\{X-X2\}), \tag{C-17}$$

$$F'(X) = Y2[B\{\exp(B\langle X-X2\rangle)\}] - C5. \tag{C-18}$$

Hence,

$$XM = \frac{1}{B}\,[\ln(C5/B) - A], \tag{C-19}$$

where

$$A = [\ln Y2-(B)(X2)]. \tag{C-20}$$

D. Determination of XM for Scheme 5. Consider Eq. (C-5) in the form

$$Y = (A)(X^B), \tag{C-21}$$

where

$$\ln A = \frac{(\ln Y2)(\ln X1) - (\ln Y1)(\ln X2)}{\ln(X1/X2)} \tag{C-22}$$

and

$$B = \ln(Y1/Y2)/\ln(X1/X2) = C2/C1. \tag{C-23}$$

We show that this reduces to Eq. (C-5) by substitution:

$$\ln Y = \frac{(\ln Y2)(\ln X1) - (\ln X1)(\ln X2)}{\ln(X1/X2)} + \{\ln(Y1/Y2)/\ln(X1/X2)\}\ \ln X. \tag{C-24}$$

Hence,

$$Y = \exp\ \frac{(\ln Y2)(\ln X1) - (\ln Y1)(\ln X2) + \ln(Y1/Y2)\ \ln X}{\ln(X1/X2)}\ , \tag{C-25}$$

$$= Y2\ \exp\ \frac{\ln(X/X2)\ \ln(Y1/Y2)}{\ln(X1/X2)} \tag{C-26}$$

Hence, the form of Eqs. (C-21) through (C-23) is equivalent to Eq. (C-5). Therefore, using the former description, and constructing the functional difference we arrive at

$$F(X) = (A)(X^B) - [Y2 + C5(X-X2)]. \tag{C-27}$$

Therefore

$$F'(X) = (A)(B)\ X^{B-1} - C5 \tag{C-28}$$

and

$$XM = [C5/(A)(B)]^{[1/(B-1)]}\ . \tag{C-29}$$

In order to avoid computational difficulties, this is calculated conveniently as for $B < 3$

$$XM = \exp\left\{\frac{1}{B-1}\ \ln\left[\left(\frac{Y1-Y2}{Y1}\right)\left(\frac{1}{B}\right)\frac{(X1)^B}{(X1-X2)}\right]\right\}\ , \tag{C-30}$$

for $B \geq 3$

$$XM = \exp\left\{\frac{1}{B-1}\ln\left[\left(\frac{Y1-Y2}{(X1-X2)B}\right)\right.\right.$$

$$\left.\left. - \left[(\ln Y2)(\ln X1) - (\ln Y1)(\ln X2)\right]/\ln(X1/X2)\right]\right\}\ . \tag{C-31}$$

APPENDIX D

DERIVATION OF KERNEL BROADENING EQUATIONS

I. Theory

The general Doppler broadening equation is written as[50,51]

$$\sqrt{E}\sigma(E,T) =$$

$$= \frac{1}{2}\sqrt{\frac{\alpha}{\pi E}}\int_0^\infty [\sqrt{E_r}\ \sigma(E_r,0)]\left\{e^{-\alpha(\sqrt{E} - \sqrt{E_r})^2}\right.$$

$$\left. - e^{-\alpha(\sqrt{E} + \sqrt{E_r})^2}\right\}\ , \tag{D-1}$$

with the following notations for the derivation

m = projectile mass (e.g., neutron, proton, alpha, etc.),
$\vec{V}$ = projectile velocity,
V = $|\vec{V}|$ = projectile speed,
E = $\frac{1}{2}mV^2$ = projectile energy,
M = target nuclei mass,
$\vec{V}_T$ = target velocity,
V_T = $|\vec{V}_T|$ = target speed,
E_T = $\frac{1}{2}MV_T^2$ = target energy,
A = M/m = atomic weight ratio (target mass/projectile mass),
$\vec{V}_r$ = $\vec{V} - \vec{V}_T$ = relative velocity,
V_r = $|\vec{V}_r|$ = relative speed,
E_r = $\frac{1}{2}mV_r^2$ = relative energy of the neutron as "seen" by the target,
$\sigma(V,0)$ = cold (0°K) cross section,
$\sigma(V,T)$ = Doppler-broadened cross section,
$R(V,T)$ = $V\sigma(V,T)$ = reaction rate (per neutron),
$P(\vec{V}_T)d\vec{V}_T$ = normalized target-nuclei velocity distribution,
α = A/KT, and
K = Boltzmann's constant .

The Doppler broadening equation can be slightly generalized by recognizing that it may be used not only to broaden cross sections from 0 K to temperature T K, but may also be used to broaden cross sections from any temperature T_1 K to any higher temperature T_2 K. Thus, Eq. (D-1) is generalized to

$$\sqrt{E}\sigma(E,T_2) =$$

$$= \frac{1}{2}\sqrt{\frac{\alpha}{\pi E}} \int_0^\infty [\sqrt{E_r}\sigma(E_r,T_1)]$$

$$\times \left\{e^{-\alpha(\sqrt{E} - \sqrt{E_r})^2} - e^{-\alpha(\sqrt{E} + \sqrt{E_r})^2}\right\} dE \quad , \qquad \text{(D-2)}$$

where

$$\alpha = \frac{A}{k(T_2 - T_1)} \quad . \tag{D-3}$$

Defining for convenience

$$y^2 = \sigma E = \beta V^2 \ , \tag{D-4}$$

$$x^2 = \alpha E_r = \beta V_r^2 \quad .$$

The Doppler broadening equation becomes

$$\sigma(y,T_2) = \frac{1}{y^2}\sqrt{\frac{1}{\pi}}\int_0^\infty x^2\sigma\left(x,T_1\right)\left\{e^{-(x-y)^2} - e^{-(x+y)^2}\right\} dx \ . \tag{D-5}$$

The ensuing development[29] can be simplified by defining

$$\sigma^*(y,T_2) = \frac{1}{y^2}\sqrt{\frac{1}{\pi}}\int_0^\infty x^2\sigma(x,T_1)e^{-(x-y)^2}\ dy. \tag{D-6}$$

and noting that the Doppler-broadened cross section is

$$\sigma(y,T_2) = \sigma^*(y,T_2) - \sigma^*(-y,T_2) \quad . \tag{D-7}$$

Recognizing that the tables of energy vs cross section use linear-linear interpolation between tabulated values (see 3.1 and 4.1), the cross section is given as

$$\sigma(E,T_1) = \left[\frac{E - E_k}{E_{k+1} - E_k}\right]\sigma_{k+1} + \left[\frac{E_{k+1} - E}{E_{k+1} - E_k}\right]\sigma_k : \quad E\varepsilon(E_k,E_{k+1}) \tag{D-8}$$

$$= A_k + B_k E \ ,$$

$$\sigma(X,T_1) = A_k + C_k x^2 : \ x\varepsilon(x_k,X_{k+1}) \quad . \tag{D-9}$$

Since tabulated cross sections span only a finite energy range (e.g., 10^{-5} eV to 20 MeV), the cross section is arbitrarily continued as constant outside the range. Inserting Eq. (D-8) into Eq. (D-6), one obtains

$$\sigma^*(y,T_2) = \frac{1}{y^2}\sqrt{\frac{1}{\pi}} \sum_k \int_{x_k}^{x_{k+1}} x^2[A_k + C_k x^2]\, e^{-(x-y)^2}\, dx \,. \tag{D-10}$$

By changing variables, let $Z = x - y$, and collect terms in powers of Z

$$\sigma^*(y,T_2) = \frac{1}{y^2}\sqrt{\frac{1}{\pi}} \sum_k \int_{x_k-Y}^{x_{k+1}-y} \left[C_k Z^4 + 4C_k y Z^3 + \left(A_k + 6C_k y^2\right) Z^2 \right.$$

$$\left. + \left(2A_k y + 4C_k y^3\right) Z + \left(A_k y^2 + C_k y^4\right)\right] e^{-Z^2} dZ \,, \tag{D-11}$$

which can be defined exactly in terms of the functions

$$H^n(a,b) = F^n(a) - F_n(b): \quad n = 0,1,2,3,4 \,, \tag{D-12}$$

$$F^n(a) = \frac{2}{\sqrt{\pi}} \int_0^a z^n e^{-Z^2}\, dZ. \tag{D-13}$$

These functions can be easily shown to satisfy the recursion relationship

$$F_n(a) = \frac{(n-1)}{2} F^{n-2}(a) - \sqrt{\frac{1}{\pi}}\, a^{n-1} e^{-a^2} + \sqrt{\frac{1}{\pi}}\, \delta_{0,n-1} \,. \tag{D-14}$$

By explicitly evaluating Eq. (D-13) for m = 0 and 1, as well as by applying the relationship, the required functions are

$$F^0(a) = \mathrm{ERF}(a) \,, \tag{D-15}$$

$$F^1(a) = \sqrt{\frac{1}{\pi}}\,(1 - e^{-a^2}) \,, \tag{D-16}$$

$$F^2(a) = \frac{1}{2}\,\mathrm{ERF}(a) - \frac{a}{\sqrt{\pi}}\,e^{-a^2}\quad , \tag{D-17}$$

$$F^3(a) = \sqrt{\frac{1}{\pi}}\left[1 - (1 + a^2)e^{-a^2}\right], \text{ and} \tag{D-18}$$

$$F^4(a) = \frac{3}{4}\,\mathrm{ERF}(a) - \sqrt{\frac{1}{\pi}}\left(\frac{3a}{2} + a^3\right)e^{-a^2}\quad . \tag{D-19}$$

With the definition of these functions, the algorithm describing the Doppler-broadened cross section at any arbitrary energy is complete.

II. Optimization and Implementation of the SIGMA1 Technique

The SIGMA1 Doppler-broadening method may be optimized both at the program design level and at the operating procedures level.

At the program design level, the exact evaluation of the Doppler-broadened cross section can be obtained with the proposed algorithm, but it can be a costly procedure since the calculational time can vary as the square of the number of points used to represent a given reaction. Furthermore, even though the solution via the SIGMA1 method can be expressed in terms of known functions (i.e., ERF(x) and e^{-x^2}), it is potentially subject to round-off error since the solution is given in terms of many differences of these functions [e.g., $F_n(a) - F_n(b)$].

The strongly convergent Gaussian character of the Doppler-broadening kernel can be used to truncate the Doppler-broadening integral. Because of the exponential term $e^{-(x-y)^2}$ [see Eq. D-5)], the major contribution to the integral will come from the region where x is close to y. Therefore, instead of extending the integral from $x\varepsilon(0,\infty)$ it may be truncated to an integral centered about y, $x\varepsilon(y - N, y + N)$. The TEMPO program[52] uses $N = \sqrt{8}$ because $\mathrm{ERFC}(\sqrt{8}) \sim 10^{-4}$. However, the truncation procedure should recognize that although $e^{-(x-y)^2}$ is rapidly decreasing, the term $x^2\sigma(x,T)$ may be rapidly increasing, particularly the cross section in the resonance region. Therefore, the truncation procedure should be

$$\int_0^{\infty} x^2\,(x,T)e^{-(x-y)^2}\,dx = \int_{y-N}^{y+N} x^2\,(x,T)e^{-(x-Y)^2}\,dx + R(y), \tag{D-20}$$

$$R(y) = \int_0^{y-N} x^2\alpha(x,T)e^{-(x-y)^2}\,dx + \int_{y+N}^{\infty} x^2\alpha(x,T)e^{-(x-y)^2}\,dx < \varepsilon, \qquad \text{(D-21)}$$

$$R(y) < 2\,\langle\sigma\rangle \int_N^{\infty} (Z + y)^2\, e^{-Z^2}\,dZ \quad . \qquad \text{(D-22)}$$

Allowing for a variation in cross section of four orders of magnitude (10^4) and using an allowable error of 0.1%, which is well below what can be experimentally measured presently or in the foreseeable future, the integral can be safely truncated using N = 4.

Therefore, the truncated integral should be extended only over those intervals in which at least one end is within four units of y. In particular, the second term $\sigma^*(-y,T_2)$ [Eq. (D-7)] need not be calculated unless $y \leq 4$.

III. Calculation of Integrals

There are many algorithms available to calculate ERF(X)[54,55] to high precision. However, it must be recognized that although most calculate ERF(X) to some desired degree of accuracy, one can experience precision difficulties in solving for ERF(a) - ERF(b), for a close to b. Cullen[29] has suggested tabulation of functional values (and successive derivatives) at fixed nodes (energy points) prior to the Doppler broadening operation and interpolation in the tables during execution. MacFarlane and Hancock[56] have used a direct expansion of the defining integral for $H^m(a,b)$. Neither is implemented in the current version of MINX; therefore, broadening is not performed for energies below 0.1 eV. Finally, the bootstrapping procedure [Eq. (D-2)] referred to above, which is currently implemented, dramatically reduces the number of integral calculations required since the procedure begins, in each case, with successively fewer points.

APPENDIX E

POINT CROSS-SECTION THINNING

The thinning procedure[27] is logically equivalent to the process of linearization since one starts with a function f(E) which is given as a table of values and a linear interpolation law between the tabulated values, and one tries to determine a function $\bar{f}(E)$, such that:

(a) $\bar{f}(E)$ is also a table of values and linear interpolation laws,

(b) The fractional difference between the "exact" f(E) and the approximation $\bar{f}(E)$ is less than some desired allowable error ε for all energies,

i.e., $|f(E) - \bar{f}(E)| < \varepsilon f(E)$.

However, an additional criterion is added:

(c) The tabulated values of $\bar{f}(E)$ must constitute the smallest possible subset of the tabulated values in f(E). Thus, all values in the tabulation of f(E) that can be approximated (to within ε) by linear interpolation between adjacent points must be eliminated.

The following multipoint algorithm has been developed for thinning data files.

(a) The first and third point of a table are selected and a test is made to determine whether point number two can be approximated by linear interpolation between points 1 and 3.

(b) If the test is successful the test interval is extended to include point 4, and again, points 2 and 3 are tested to see whether they can be approximated by an interpolation between points 1 and 4.

(c) Generalizing to N points, if the points 2, 3, ...(N-1) can be approximated by interpolating between points 1 and N, the algorithm proceeds to N + 1 points.

(d) If any one (or more) of the points 2, 3, ...(N-1) fail the interpolation test between points 1 and N, the test interval has been extended too far. However, since the previous test (with N-1 points) must have been successful for the algorithm to reach this far, all the points between 1 and N-1 can be removed, leaving only the end points 1 and N-1. The algorithm is repeated with points N-1 and N + 1.

The multipoint algorithm is considerably different from the three-point thinning technique used in the earlier versions of the ENDF/B system routine CROP.[57]

The three-point algorithm operates by discarding point 2 if it can be interpolated between the adjacent points 1 and 3, then proceeds to test point 3 by interpolating between points 1 and 4. If point 3 is rejected, there remains no guarantee that point 2, which was rejected earlier, can be obtained by interpolating between the remaining points 1 and 4. This method produces particularly erroneous results when thinning points located very closely on a slowly varying smooth curve. The multipoint thinning algorithm is not limited to linear tables but can be used with any interpolation law. A generalized version has been implemented in SIGMA1.

APPENDIX F

EFFECTIVE CROSS-SECTION GENERATION PROCEDURES TAKEN FROM THE ETOX[5] CODE

I. THEORY

Unresolved calculations follow closely the methods and approximations used in the MC[2] code,[30] where infinitely dilute and self-shielded cross sections are calculated at discrete energy points E* in the unresolved energy region.

The infinitely dilute and self-shielded cross sections are given as

$$\langle\sigma_s(E^*)\rangle = \frac{\int_{E_1}^{E_2} \frac{\sigma_x(E,T)\,dE}{E}}{\int_{E_1}^{E_2} \frac{dE}{E}} \qquad (x = f,c,e) \quad , \tag{F-1}$$

$$\overline{\sigma_x(E^*)} = \frac{\int_{E_1}^{E_2} \frac{\sigma_x(E,T)dE}{[\sigma_t(E,T) + \sigma_o]E}}{\int_{E_1}^{E_1} \frac{dE}{[\sigma_t(E,T) + \sigma_o]E}} \quad , \tag{F-2}$$

and

$$\overline{\sigma_t(E^*)} = \frac{\int_{E_1}^{E_2} \frac{dE}{[\sigma_t(E,T) + \sigma_o]E}}{\int_{E_1}^{E_2} \frac{dE}{[\sigma_t(E,T) + \sigma_o]^2 E}} - \sigma_o, \tag{F-3}$$

where E* is some energy point in the energy range (E_1,E_2) which is assumed to contain many narrow resonances. The symbol X stands for either fission, elastic, or capture cross sections. Note that the braces imply infinitely dilute cross sections [flux representation including only the gross (1/E) behavior] whereas bar superscripts indicate self-shielded cross sections (i.e., flux representation includes inverse cross-section type of weighting). Equations (F-1) through (F-3) are simplified if one assumes that the energy variation in the integrands in the above integrals only occurs in the rapidly varying resonance parts of the ψ function. The slowly varying terms are evaluated at the energy E*. In this approximation the elastic cross section, for example, is written as*

*As in the MC^2 code,[30] the interference-scattering term in the elastic cross section is ignored.

$$\sigma_e(E,E^*,T) = \sum_{s=1}^{N} \sum_{r=1}^{N_s} \frac{\sigma_{o_r}^s(E^*)\Gamma_{e_r}^s(E^*)}{\Gamma_r^s(E^*)} \psi\left[\xi_r^s(E^*), 2(E - E_r^s)/\Gamma_r^s(E^*)\right]$$

$$+ \sigma_p(E^*) + \sigma_{e_F}(E^*) \quad . \qquad \text{(F-4)}$$

The above assumption should be a good approximation since in the unresolved region the energy interval $(E_2 - E_1)$ may be picked to be small with respect to variations in the slowly varying components of the cross section. The notations used in Eq. (F-4) correspond to

s : spin state (of a given J),

r : summation over all resonances with spin state s,

$\sigma_{o_r}^s(E^*)$: peak cross section evaluated at energy E*,

$\Gamma_e^s(E^*)$: neutron width evaluated at energy E*,

$\Gamma_r^s(E^*)$: total width evaluated at energy E*,

$\psi(\xi,\chi)$: Doppler broadened line shape function,

$\xi_r^s(E^*)$: $\Gamma_r^s(E^*)/(4E^*kT/M)^{1/2}$,

K : Boltzmann constant,

M : atomic weight ratio for the target,

$\sqrt{4E^*kT/M}$: Doppler width evaluated at energy E*,

$\sigma_p(E^*)$: potential scattering cross section,

$\sigma_{e_F}(E^*)$: File 3 "floor correction" to resonance structure.

With this approximation, Eqs. (F-1) - (F-3) become

$$\langle\sigma_x(E^*)\rangle = \frac{1}{E_2 - E_1}\int_{E_1}^{E_2}\sum_s\sum_r \sigma^s_{x_r}(E,E^*)dE + \sigma_{x_F}(E^*) + \sigma_p(E^*)\delta_{x_e} \quad ,(F\text{-}5)$$

$$\overline{\sigma_x(E^*)} = \left[\int_{E_1}^{E_2} \frac{\sum_s\sum_r \sigma^s_{x_r}(E,E^*)dE}{\left(\sum_s\sum_r \sigma^s_{t_r}(E,E^*) + \bar{\sigma}_p\right)} \Bigg/ \right.$$

$$\left. \int_{E_1}^{E_2} \frac{dE}{\left(\sum_s\sum_r \sigma^s_{t_r}(E,E^*) + \bar{\sigma}_p\right)}\right] + \sigma_{x_F}(E^*) + \sigma_p(E^*)\delta_{x_e}, \qquad (F\text{-}6)$$

$$\overline{\sigma_t(E^*)} = \left[\int_{E_1}^{E_2} \frac{dE}{\sum_s\sum_r \sigma^s_{t_r}(E,E^*) + \bar{\sigma}_p} \Bigg/ \right.$$

$$\left. \int_{E_1}^{E_2} \frac{dE}{\sum_s\sum_r \left[\sigma^s_{t_r}(E,E^*) + \bar{\sigma}_p\right]^2}\right] - \sigma_0 \qquad (F\text{-}7)$$

Note that the expression for the effective total cross section is different in form than elastic, fission, or capture due to its direct relation to the transport cross section. This matter is described more fully in Appendix A of the ETOX[5] report, where

$$\bar{\sigma}_p = \sigma_p(E^*) + \sigma_{f_F}(E^*) + \sigma_{c_F}(E^*) + \sigma_{e_F}(E^*) + \sigma_o \qquad \text{(F-8)}$$

is the potential scattering cross section including contributions of "background" cross sections from File 3.

With the assumption of many resonances in the interval $(E_2 - E_1)$, the resonance contributions in the above integrals are treated statistically. The interval $(E_2 - E_1)$ is replaced by D^s, the average spacing of the resonances of sequence s, multiplied by the number N^s contained in the interval. The summation over resonances in a given sequence is then replaced with a double integration over a Porter-Thomas (chi-squared) distribution with n and m degrees of freedom. Symbolically

$$\frac{1}{N^s}\sum_r f_r^s \rightarrow \int_0^\infty \int_0^\infty P_{n^s}(y)P_{m^s}(z)f^s(y,z)\,dy\,dz \equiv \langle f^s \rangle_p \quad , \qquad \text{(F-9)}$$

where

$$P_n(y) = \frac{n}{2}\frac{1}{\Gamma\left(\frac{n}{2}\right)}\left(\frac{ny}{2}\right)^{\frac{n}{2}-1}\exp\left(-\frac{ny}{2}\right) . \qquad \text{(F-10)}$$

The function f represents the formulation for the cross section in terms of elastic widths and fission widths, (for a given sequence s) where the width distributions are represented according to Eq. (F-10) with n and m degrees of freedom, respectively

$$\Gamma_e^s(E^*,y) = y\Gamma_e^s(E^*) \quad , \qquad \text{(F-11)}$$

$$\Gamma_f^s(E^*,z) = z\Gamma_f^s(E^*) \quad . \tag{F-12}$$

With the above replacements and the narrow resonance approximation such that

$$\int_{E_1}^{E_2} f(E)dE \rightarrow \int_{-\infty}^{\infty} f(E)dE, \tag{F-13}$$

Eq. (F-5) becomes

$$\langle\sigma_x(E^*)\rangle = \sum_s \frac{1}{D_s} \langle\Gamma_r^s(E^*)\sigma_o^s(E^*) \int_o^{\infty} \psi(\xi^s,\chi)d\chi\rangle_P$$

$$+ \sigma_{x_F}(E^*) + \sigma_p(E^*)\delta_{x_e} \quad . \tag{F-14}$$

Since

$$\int_o^{\infty} \psi(\xi^s,\chi)d\chi = \frac{\pi}{2} \quad , \tag{F-15}$$

independent of the value of ξ^s, the infinite dilute cross section is finally given as

$$\langle\sigma_x(E^*)\rangle = \frac{\pi}{2} \sum_s \frac{1}{D_s} \langle\sigma_o^s(E^*)\Gamma_x^s(E^*)\rangle_P$$

$$+ \sigma_{x_F}(E^*) + \sigma_p(E^*)\delta_{x_e} \quad . \tag{F-16}$$

Equation (F-16) is the equation used in MINX to derive unresolved infinitely dilute cross sections for elastic, capture and fission. (The total here is the sum of the parts.)

Due to the appearance of the resonance terms in the denominator of the expressions in Eqs. (F-6) and (F-7) the self-shielded cross sections require additional approximations and analysis for their evaluation. Consistent with the narrow resonance approximation, it is assumed that overlap effects between different resonances of the same sequence and overlap between different sequences may be ignored. The numerator, for example, in Eq. (F-6) then becomes

$$\mathrm{NUM} = \sum_s \sum_r \int_{E_1}^{E_2} \frac{\sigma^s_{x_r}(E,E^*)}{\sigma^s_{t_r}(E,E^*) + \bar{\sigma}_p} \left[1 - \sum_{s' \neq s} \sum_{r'} \frac{\sigma^{s'}_{t_{r'}}(E,E^*)}{\left(\sigma^s_{t_{r'}}(E,E^*) + \bar{\sigma}_p\right)} \right] dE \,. \qquad \text{(F-17)}$$

Rewriting Eq. (F-17) in terms of the line-shape functions $\psi(\xi^s_r, \chi^s_r)$ gives

$$\mathrm{NUM} = \sum \sum \frac{\Gamma^s_{x_r}(E^*)}{\Gamma^s_r(E^*)} \int_{E_1}^{E_2} \frac{\psi(\xi^s_r,\chi^s_r)}{\psi(\xi^s_r,\chi^s_r) + \beta^s_r} \left[1 - \sum_{s' \neq s} \sum_{r'} \frac{\psi(\xi^{s'}_{r'},\chi^{s'}_{r'})}{\psi(\xi^{s'}_{r'},\chi^{s'}_{r'}) + \beta^{s'}_{r'}} \right] dE, \qquad \text{(F-18)}$$

where

$$\beta_r^s = \bar{\sigma}_p / \sigma_{o_r}^s (E^*). \tag{F-19}$$

The sequences s' are uncorrelated with respect to s in Eq. (F-18). Consequently, it is necessary to integrate the primed summations over the probability of finding resonance r' of s' at a separation δ from resonance r of s, where δ ranges from $-(E_r - E_1)$ to $(E_2 - E_r)$ and E_r is the location of the resonance r in the interval $E_2 - E_1$. With this and the statistical analysis following Eq. (F-7), Eq. (F-18) is given as[34]

$$\text{NUM} = (E_2 - E_1) \sum_s \frac{\langle \Gamma_r^s(E^*) J(\xi^s, \beta^s) \rangle_p}{D_s}$$

$$\left[1 - \sum_{s' \neq s} \frac{\langle T^{s'}(E^*) J(\xi^{s'}, \beta^{s'}) \rangle_p}{D_{s'}} \right] , \tag{F-20}$$

where the usual J integral is defined as

$$J(\xi^s, \beta^s) \equiv \int_0^\infty \frac{\psi(\xi^s, \chi) d\chi}{\psi(\xi^s, \chi) + \beta^s} . \tag{F-21}$$

The denominator in Eq. (F-6) and the terms in Eq. (F-7) are evaluated in a similar manner as that given above for the numerator in Eq. (F-6). The final expressions for the self-shielded cross sections available in MINX are

$$\overline{\sigma_x(E^*)} = \bar{\sigma}_p \sum_s a_x^s \left(1 - \sum_{s' \neq s} b^{s'} \right) \Bigg/ \left[1 - \sum_s b^s \left(1 - \sum_{s' \neq s} b^{s'} \right) \right]$$

$$+ \sigma_{x_F} + \sigma_p \delta_{x_e} , \tag{F-22}$$

$$\overline{\sigma_t(E^*)} = \bar{\sigma}_p \left[1 - \sum_s b^s \left(1 - \sum_{s' \neq s} b^{s'}\right)\right] \Bigg/ \left[1 - \sum_s c^s \left(1 - \sum_{s' \neq s} c^{s'}\right)\right] - \sigma_o \ , \qquad \text{(F-23)}$$

where

$$a_x^s = \langle \Gamma_x^s J^s \rangle_p / D_s , \qquad \text{(F-24)}$$

$$b^s = \langle \Gamma^s J^s \rangle_p / D_s \ , \qquad \text{(F-25)}$$

$$c^s = \langle \Gamma^s K^s \rangle_p / D_s \ , \text{ and} \qquad \text{(F-26)}$$

$$K^s = K(\xi^s, \beta^s) = \int_0^\infty \frac{\psi(\xi^s, \chi)[\psi(\xi^s, \chi) + 2\beta^s]}{[\psi(\xi^s, \chi) + \beta^s]^2} \, dX \ . \qquad \text{(F-27)}$$

II. Program Details for the Unresolved Calculations

The calculations of the J and K integrals and the statistical brackets $\langle \ \rangle_p$ use the methods given in the MC^2 code.[30]

The J and K integrals are evaluated by breaking the infinite interval into two finite intervals plus a remainder term. In particular, the code assumes

$$J(\beta,\xi) = \int_0^{\infty} \frac{\psi(\xi,\chi)}{\psi(\xi,\chi) + \beta}\, d\chi$$

$$= \int_0^{20/\xi} \frac{\psi}{\psi + \beta}\, d\chi$$

$$+ \int_{20/\xi}^{200/\xi} \frac{\psi}{\psi + \beta}\, d\chi + \text{REMJ}, \qquad \text{(F-28)}$$

where

$$\psi(\xi,\chi) \xrightarrow[\xi\chi >> 1]{} \frac{1}{1 + X^2}\ , \qquad \text{(F-29)}$$

$$\text{REMJ} = \int_{200/\xi}^{\infty} \frac{\psi}{\psi + \beta}\, d\chi\ ,$$

$$\frac{1}{\beta} \int_{200/\xi}^{\infty} \frac{dX}{(a^2 + X^2)} = \frac{1}{\beta a}\left(\frac{\pi}{2} - \tan^{-1}\frac{200}{\xi a}\right), \text{ and} \qquad \text{(F-30)}$$

$$a = \sqrt{\frac{1+\beta}{\beta}} \,. \tag{F-31}$$

$$K(\beta,\xi) = \int_0^\infty \frac{\psi(\psi+2\beta)}{(\psi+\beta)^2} d\chi = J(\beta,\xi) + \int_0^\infty \frac{\beta\psi}{(\psi+\beta)^2}\, d\chi$$

$$= J(\beta,\xi) + \int_0^{20/\xi} \frac{\beta\psi}{(\psi+\beta)^2}\, d\chi$$

$$+ \int_{20/\xi}^{200/\xi} \frac{\beta\psi}{(\psi+\beta)^2}\, d\chi + \text{REMK} \,, \tag{F-32}$$

where

$$\text{REMK} \simeq \frac{1}{2a^2} \left((1+a^2)\ \text{REMJ} - \frac{1}{\beta a} \frac{(1-a^2)(200/a\xi)}{[(200/a\xi)^2 + 1]} \right) . \tag{F-33}$$

The integrals in the above equations are calculated using 16-point Gaussian quadrature.

APPENDIX G

CHOICE OF WITHIN-GROUP WEIGHTING FLUX FOR MINX

The group-averaged cross sections produced by MINX are defined by

$$\sigma_{xng} = \frac{\int_g \sigma_x(E)\phi_n(E)dE}{\int_g \phi_n(E)dE} \qquad \text{(G-1)}$$

where $\sigma_x(E)$ is the energy-dependent cross section for reaction x and $\phi_n(E)$ is a Legendre component of the neutron angular flux. Since MINX attempts to produce a set of cross sections independent of the composition and arrangement of any particular problem, some assumptions have to be made about the nature of the flux components required for these averages. Coarse variations in the flux may be accounted for by using fine energy groups. MINX assumes that the fine variations of the flux within each energy group can be adequately represented by the narrow resonance approximation and the B_0 approximation, and that the cross sections will be used in a system large with respect to the neutron mean-free path. It is further assumed that the only important features of the flux are those which correlate with features in the cross section being averaged. The result is the Bondarenko flux model[19]

$$\phi_n(E) = \frac{W_n(E)}{[\Sigma_t(E)]^{n+1}} \propto \frac{W_n(E)}{[\sigma_o + \sigma_t(E)]^{n+1}} , \qquad \text{(G-2)}$$

where $W_n(E)$ is a weight function which varies slowly with energy, Σ_t is the total macroscopic cross section, σ_t is the total microscopic cross section for the isotope of interest, and σ_0 is a parameter called the "background cross section per atom" which is assumed to be constant within the energy range of any group. This single parameter can be used to allow for mixture and heterogeneity effects in many practical situations.[10]

Using this flux model, the formula for the multigroup cross sections becomes

$$\sigma_{xn,g}(T,\sigma_o) = \frac{\int_g \frac{\sigma_x(E,T)}{[\sigma_o + \sigma_t(E,T)]^{n+1}} W_n(E)dE}{\int_g \frac{1}{[\sigma_o + \sigma_t(E,T)]^{n+1}} W_n(E)dE} \quad . \tag{G-3}$$

In the unresolved resonance energy range, the explicit dependence of cross section on energy is not known. The integrands are replaced by their expected values

$$\sigma_{xn,g}(T,\sigma_o) = \frac{\int_g \left\langle \frac{\sigma_x}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle W_n dE}{\int_g \left\langle \frac{1}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle W_n dE} \quad , \tag{G-4}$$

where the expected values are averages over the distributions of resonance positions and widths expected in the vicinity of energy E. Defining average self-shielded cross sections with respect to those distributions ,

$$\langle \sigma_x \rangle_n \equiv \frac{\left\langle \frac{\sigma_x}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle}{\frac{1}{\langle [\sigma_o + \sigma_t]^{n+1} \rangle}} \quad . \tag{G-5}$$

Noting that these are the quantities produced by the UNRESR module,

$$\langle\sigma_t\rangle_n = \frac{\left\langle \frac{\sigma_o + \sigma_t - \sigma_o}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle}{\left\langle \frac{1}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle} = \frac{\left\langle \frac{1}{[\sigma_o + \sigma_t]^{n}} \right\rangle}{\left\langle \frac{1}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle} - \sigma_o \quad ,$$

$$\left\langle \frac{1}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle = \frac{\left\langle \frac{1}{[\sigma_o + \sigma_t]^{n}} \right\rangle}{\sigma_o + \langle\sigma_t\rangle^n} \quad , \text{ and}$$

$$\left\langle \frac{1}{[\sigma_o + \sigma_t]^{n+1}} \right\rangle = \prod_{k=o}^{n} \frac{1}{\sigma_o + \langle\sigma_t\rangle_k} \quad , \tag{G-6}$$

the multigroup cross section in the unresolved region can be written as

$$\sigma_{xn,g}(T, \sigma_o) = \frac{\int_g \langle\sigma_t(T,\sigma_o)\rangle_n \prod_{k=o}^{n} \frac{1}{\sigma_o + \langle\sigma_t(T,\sigma_o)\rangle_k} W_n(E)dE}{\int_g \prod_{k=o}^{n} \frac{1}{\sigma_o + \langle\sigma_t(T,\sigma_o)\rangle_k} W_n(E)dE} \cdot \tag{G-7}$$

The form of Eq. (G-7) is very similar to that of Eq. (G-3), except that the cross sections have been replaced by self-shielded averages.

APPENDIX H

ISOTXS AND BRKOXS FORMAT DESCRIPTION[23]

I. ISOTXS - Nuclide-Ordered Neutron Cross Sections

Revisions in this file affect the fission yield matrices (CHI data), and the transport and total cross sections. An optional number of vector fission-yield spectra may be defined where each spectrum may be assigned to any incident group. In practice, this reduces the CHI matrix to a rectangular matrix requiring greatly reduced storage space where a large number of groups are involved. The variable blocking provided on the Version II full CHI matrix is, therefore, no longer required in the Version III formulation.

P_ℓ weighted transport and total cross-section arrays

$$\sigma^G_{tr_\ell} = \sigma^G_{t_\ell} - \sum_{G'} \sigma^{G\to G'}_{S_\ell} \qquad \ell=1,\ldots,\text{LTRN} \tag{H-1}$$

$$\sigma^G_{t_\ell} = \frac{\int_G \sigma_t \phi_\ell (E)\,dE}{\bar{\phi}_\ell{}^G} \qquad \ell=0,1,\ldots,\text{LTOT} \tag{H-2}$$

are supplied in place of the derived quantities

$$\text{STRSN} = \sigma^G_{t_0},\ \sigma^G_{t_1},\ \sigma^G_{tr_K}\ (K\leq\text{LTOT}),\ \text{or other recipe,} \tag{H-3}$$

$$\text{STRDIF} = \sigma^g_{tr_1},\ \text{and} \tag{H-4}$$

$$\text{STOT} = \sigma^G_{t_0} \tag{H-5}$$

provided in the Version II file. The P_ℓ weighted scattering cross sections

$$\sigma_s^{G\to G'} = \frac{\int_G \int_{G'} \sigma_{S_\ell}(E\to E')\,\phi_\ell(E)\,dE'\,dE}{\bar{\phi}_\ell^G} \qquad \text{(H-6)}$$

are now given in the file scattering blocks instead of derived matrices. The only difference in the old and new scattering blocks is in in-group terms for S_n applications which formerly contained

$$\sigma_{S_\ell}^{G\to G} + \sigma_{t_0}^G - \sigma_{t_\ell}^G,\ \ell=0,1,\ldots,L\ ,$$

$$\sigma_{S_\ell}^{G\to G} + \sigma_{t_1}^G - \sigma_{t_\ell}^G,\ \ell=0,1,\ldots,L\ ,$$

or

$$\sigma_{S_\ell}^{G\to G} + \sigma_{tr_K}^G - \sigma_{t_0}^G,\ \ell=0,1,\ldots,K-1\ ,$$

respectively, depending upon the approximation used in STRSN. In Version III, the in-group terms in the file are simply $\sigma_{S_\ell}^{G\to G}$, consequently, transport approximations as in equation (H-7) are left as options to be provided in flux codes.

Data added to ISOTXS include identifiers for the cross-section data source such as ENDF/B, the capture thermal energy yield, and coordinate-dependent transport cross sections. The identifiers, HIDENT and HMAT, the capture energy, ECAPT, and the number of coordinate directions, ISTRPD, for which coordinate-dependent transport cross sections are given, have been added to the Isotope Control and Group Independent Data record. The new coordinate-dependent transport cross sections are contained in the PRINCIPAL CROSS SECTIONS record.

Some problems arise in the interpretation of the vectors IDSCT(N) and LORD(N) in the ISOTOPE CONTROL AND GROUP INDEPENDENT DATA record. IDSCT(N) specifies the identity and ordering of scattering blocks, and LORD(N) specifies the number

of orders contained in each block N. Elaborate sorting would be required to use the data if the most general interpretation of IDSCT(N) and LORD(N) is made. However, it seems reasonable to assume that the data will always be logically ordered.

Considerable programming convenience is achieved if the same IDSCT vector is used on all isotopes. At least one would expect to find a consistent ordering of the types of cross sections, total, elastic, inelastic, and n,2n, and would expect to find all the cross sections for a given type contained in contiguous blocks. We note that any given type may be deleted in an isotope either by setting the appropriate LORD(N)=0 or by omitting the pertinent blocks in IDSCT. One would expect in the latter case, however, the ordering of types to be preserved except for the deletions.

Similarly, one would expect the ordering and blocking of cross-section orders, except for deletions, to be consistent over all the isotopes.

Finally, one would not expect to find sub-blocking used (NSBLOK) if the individual major blocks defined by IDSCT and LORD contain more than one order.*

```
C*****************************************************************************
C                       REVISED 07/01/73                                      *
C                                                                             *
CF          ISOTXS-III                                                        *
CE          MICROSCOPIC GROUP NEUTRON CROSS SECTIONS                          *
C                                                                             *
CN                      THIS FILE PROVIDES A BASIC BROAD GROUP                *
CN                      LIBRARY, ORDERED BY ISOTOPE                           *
CN                      FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES          *
CN                      ONLY.                                                 *
C                                                                             *
C*****************************************************************************


C-----------------------------------------------------------------------------*
CS          FILE STRUCTURE                                                    *
CS                                                                            *
CS             RECORD TYPE                          PRESENT IF               *
CS             ===========================          ==========               *
CS             FILE IDENTIFICATION                  ALWAYS                   *
CS             FILE CONTROL                         ALWAYS                   *
CS             FILE DATA                            ALWAYS                   *
CS             SET CHI DATA                         ICHIST.GT.1              *
CS                                                                            *
CS   *************(REPEAT FOR ALL ISOTOPES)                                  *
CS   *         ISOTOPE CONTROL AND GROUP                                      *
CS   *                      INDEPENDENT DATA        ALWAYS                   *
CS   *         PRINCIPAL CROSS SECTIONS             ALWAYS                   *
CS   *         ISOTOPE CHI DATA                     ICHI.GT.1                *
CS   *                                                                       *
CS   *  **********(REPEAT TO NSCMAX SCATTERING BLOCKS)                       *
CS   *  *  *******(REPEAT FROM 1 TO NSBLOK)                                  *
CS   *  *  *    SCATTERING SUB-BLOCK              LORD(N).GT.0               *
CS   *************                                                           *
C                                                                             *
C-----------------------------------------------------------------------------*
```

*Note that MINX uses this option - it is necessary for large group structures.

```
C-----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        *
C                                                                      *
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      *
C                                                                      *
CW    1+3*MULT                                                         *
C                                                                      *
CB    FORMAT(11H 0V ISOTXS ,A6,1H*,                                    *
CB   12A6,1H*,I6)                                                      *
C                                                                      *
CD    HNAME          HOLLERITH FILE NAME = ISOTXS = (A6)               *
CD    HUSE           HOLLERITH USER IDENTIFICATION (A6)                *
CD    IVERS          FILE VERSION NUMBER                               *
CD    MULT           DOUBLE PRECISION PARAMETER                        *
CD                       1= A6 WORD IS SINGLE WORD                     *
CD                       2= A6 WORD IS DOUBLE PRECISION WORD           *
C                                                                      *
C-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR          FILE CONTROL                                               *
C                                                                      *
CL    NGROUP,NISO,MAXUP,MAXDN,MAXORD,ICHIST,NSCMAX,NSBLOK              *
C                                                                      *
CW    8                                                                *
C                                                                      *
CB    FORMAT(4H 10 ,8I6)                                               *
C                                                                      *
CD    NGROUP         NUMBER OF ENERGY GROUPS IN SET                    *
CD    NISO           NUMBER OF ISOTOPES IN SET                         *
CD    MAXUP          MAXIMUM NUMBER OF UPSCATTER GROUPS                *
CD    MAXDN          MAXIMUM NUMBER OF DOWNSCATTER GROUPS              *
CD    MAXORD         MAXIMUM SCATTERING ORDER (MAXIMUM VALUE OF        *
CD                     LEGENDRE EXPANSION INDEX USED IN FILE).         *
CD    ICHIST         SET FISSION SPECTRUM FLAG                         *
CD                     ICHIST.EQ.0,      NO FISSION SPECTRUM           *
CD                     ICHIST.EQ.1,      SET VECTOR                    *
CD                     ICHIST.GT.1,      SET MATRIX                    *
CD    NSCMAX         MAXIMUM NUMBER OF BLOCKS OF SCATTERING DATA       *
CD    NSBLOK         BLOCKING CONTROL FOR SCATTER MATRICES.  THE       *
CD                     SCATTERING DATA ARE BLOCKED INTO NSBLOK         *
CD                     RECORDS PER SCATTERING BLOCK.                   *
C                                                                      *
C-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR          FILE DATA                                                  -
C                                                                      -
CL    (HSETID(I),I=1,12),(HISONM(I),I=1,NISO),                         -
CL   1(CHI(J),J=1,NGROUP),(VEL(J),J=1,NGROUP),                         -
CL   2(EMAX(J),J=1,NGROUP),EMIN,(LOCA(I),I=1,NISO)                     -
C                                                                      -
CW    (NISO+12)*MULT+1+NISO                                            -
CW    +NGROUP*(2+ICHIST*(2/(ICHIST+1)))                                -
C                                                                      -
CB    FORMAT(4H 2D ,1H*,11A6,1H*/       HSETID,HISONM                  -
CB   11H*,A6,1H*,9(1X,A6)/(10(1X,A6)))                                 -
CB    FORMAT(1P6E12.5)                  CHI (PRESENT IF ICHIST.EQ.1)   -
CB    FORMAT(1P6E12.5)                  VEL,EMAX,EMIN                  -
CB    FORMAT(12I6)                      LOCA                           -
C                                                                      -
CD    HSETID         HOLLERITH IDENTIFICATION OF SET (A6)              -
CD    HISONM(I)      HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6)        -
CD    CHI(J)         SET FISSION SPECTRUM (PRESENT IF ICHIST.EQ.1)     -
CD    VEL(J)         MEAN NEUTRON VELOCITY IN GROUP J (CM/SEC)         -
CD    EMAX(J)        MAXIMUM ENERGY BOUND OF GROUP J (EV)              -
CD    EMIN           MINIMUM ENERGY BOUND OF SET (EV)                  -
CD    LOCA(I)        NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR  -
CD                      ISOTOPE I.  LOCA(1)=0                          -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SET CHI DATA                                               -
C                                                                      -
CC        PRESENT IF ICHIST.GT.1                                       -
C                                                                      -
CL    ((CHI(K,J),K=1,ICHIST),J=1,NGROUP),(ISSPEC(I),I=1,NGROUP)        -
C                                                                      -
CW    NGROUP*(ICHIST+1)                                                -
C                                                                      -
CB    FORMAT(4H 3D ,1P5E12.5/(6E12.5)) CHI                             -
CB    FORMAT(12I6)                     ISSPEC                          -
C                                                                      -
CD    CHI(K,J)       FRACTION OF NEUTRONS EMITTED IN GROUP J AS A      -
CD                      RESULT OF FISSION IN ANY GROUP USING SPECTRUM K -
CD    ISSPEC         ISSPEC(I)=K IMPLIES THAT SPECTRUM K IS USED       -
CD                      TO CALCULATE EMISSION SPECTRUM FROM FISSION     -
CD                      IN GROUP I                                     -
C                                                                      -
C-----------------------------------------------------------------------
```

```
C*****************************************************************
CR          ISOTOPE CONTROL AND GROUP INDEPENDENT DATA            *
C                                                                 *
CL    HABSID,HIDENT,HMAT,AMASS,EFISS,ECAPT,TEMP,SIGPOT,ADENS,KBR,ICHI, *
CL   1IFIS,IALF,INP,IN2N,IND,INT,LTOT,LTRN,ISTRPD,                *
CL   2(IDSCT(N),N=1,NSCMAX),(LORD(N),N=1,NSCMAX),                 *
CL   3((JBAND(J,N),J=1,NGROUP),N=1,NSCMAX),                       *
CL   4((IJJ(J,N),J=1,NGROUP),N=1,NSCMAX)                          *
C                                                                 *
CR    3*MULT+17+NSCMAX*(2*NGROUP+2)                               *
C                                                                 *
CB    FORMAT(4H 0D ,3(1X,A6)/1P6E12.5/                            *
CB   1(12I6))                                                     *
C                                                                 *
CD    HABSID        HOLLERITH ABSOLUTE ISOTOPE LABEL - SAME FOR ALL   *
CD                        VERSIONS OF THE SAME ISOTOPE IN SET (A6) *
CD    HIDENT        IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA       *
CD                        CAME(E,G, ENDF/B) (A6)                    *
CD    HMAT          ISOTOPE IDENTIFICATION (E,G, ENDF/B MAT NO.) (A6) *
CD    AMASS         GRAM ATOMIC WEIGHT                              *
CD    EFISS         TOTAL THERMAL ENERGY YIELD/FISSION (W,SEC/FISS) *
CD    ECAPT         TOTAL THERMAL ENERGY YIELD/CAPTURE (W,SEC/CAPT) *
CD    TEMP          ISOTOPE TEMPERATURE (DEGREES KELVIN)            *
CD    SIGPOT        AVERAGE EFFECTIVE POTENTIAL SCATTERING IN       *
CD                        RESONANCE RANGE (BARNS/ATOM)              *
CD    ADENS         DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE  *
CD                        CROSS SECTIONS WERE GENERATED (A/BARN,CM)*
CD    KBR           ISOTOPE CLASSIFICATION                          *
CD                     0=UNDEFINED                                  *
CD                     1=FISSILE                                    *
CD                     2=FERTILE                                    *
CD                     3=OTHER ACTINIDE                             *
CD                     4=FISSION PRODUCT                            *
CD                     5=STRUCTURE                                  *
CD                     6=COOLANT                                    *
CD                     7=CONTROL                                    *
CD    ICHI          ISOTOPE FISSION SPECTRUM FLAG                   *
CD                      ICHI,EQ,0,     USE SET CHI                 *
CD                      ICHI,LQ,1,     ISOTOPE CHI VECTOR          *
CD                      ICHI,GT,1,     ISOTOPE CHI MATRIX          *
CD    IFIS          (N,F) CROSS SECTION FLAG                        *
CD                     IFIS=0, NO FISSION DATA IN PRINCIPAL CROSS   *
CD                                    SECTION RECORD               *
CD                         =1, FISSION DATA PRESENT IN PRINCIPAL    *
CD                                    CROSS SECTION RECORD         *
CD    IALF          (N,ALPHA) CROSS SECTION FLAG                    *
CD                     SAME OPTIONS AS IFIS                         *
CD    INP           (N,P) CROSS SECTION FLAG                        *
CD                     SAME OPTIONS AS IFIS                         *
CD    IN2N          (N,2N) CROSS SECTION FLAG                       *
CD                     SAME OPTIONS AS IFIS                         *
CD    IND           (N,D) CROSS SECTION FLAG                        *
CD                     SAME OPTIONS AS IFIS                         *
CD    INT           (N,T) CROSS SECTION FLAG                        *
CD                     SAME OPTIONS AS IFIS                         *
CD    LTOT          NUMBER OF MOMENTS OF TOTAL CROSS SECTION PROVIDED *
CD                     IN PRINCIPAL CROSS SECTIONS RECORD           *
CD    LTRN          NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION    *
CD                     PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD  *
CD    ISTRPD        NUMBER OF COORDINATE DIRECTIONS FOR WHICH       *
CD                     COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS *
CD                     ARE GIVEN, IF ISTRPD=0, NO COORDINATE DEPENDENT *
CD                     TRANSPORT CROSS SECTIONS ARE GIVEN,          *
```

```
CD    IDSCT(N)      SCATTERING MATRIX TYPE IDENTIFICATION FOR          *
CD                     SCATTERING BLOCK N,  SIGNIFICANT ONLY IF       *
CD                     LORD(N).GT.0                                   *
CD                     IDSCT(N)=000 + NN, TOTAL SCATTERING (SUM OF    *
CD                     ELASTIC, INELASTIC, AND N, 2N SCATTERING)      *
CD                            =100 + NN, ELASTIC SCATTERING           *
CD                            =200 + NN, INELASTIC SCATTERING         *
CD                            =300 + NN, (N,2N) SCATTERING PER EMITTED*
CD                                                       NEUTRON,    *
CD                     WHERE NN IS THE LEGENDRE EXPANSION INDEX OF THE*
CD                     FIRST MATRIX IN BLOCK N                        *
CD    LORD(N)       NUMBER OF SCATTERING ORDERS IN BLOCK N,  IF        *
CD                     LORD(N)=0, THIS BLOCK IS NOT PRESENT FOR THIS  *
CD                     ISOTOPE.  IF NN IS THE VALUE TAKEN FROM        *
CD                     IDSCT(N), THEN THE MATRICES IN THIS BLOCK      *
CD                     HAVE LEGENDRE EXPANSION INDICES OF NN,NN+1,    *
CD                     NN+2,...,NN+LORD(N)-1                          *
CD    JBAND(J,N)    SCATTERING BANDWIDTH FOR GROUP J, SCATTERING       *
CD                     BLOCK N                                        *
CD    IJJ(J,N)      POSITION OF IN-GROUP SCATTERING CROSS SECTION IN   *
CD                     SCATTERING DATA FOR GROUP J, SCATTERING BLOCK  *
CD                     N,COUNTED FROM THE FIRST WORD OF GROUP J DATA, *
C                                                                     *
C*********************************************************************
C---------------------------------------------------------------------
CR          PRINCIPAL CROSS SECTIONS                                  *
C                                                                     *
CL     ((STRPL(J,L),J=1,NGROUP),L=1,LTRN),                            *
CL    1((STOTPL(J,L),J=1,NGROUP),L=1,LTOT),(SNGAM(J),J=1,NGROUP),     *
CL    2(SFIS(J),J=1,NGROUP),(SNUTOT(J),J=1,NGROUP),                   *
CL    3(CHISO(J),J=1,NGROUP),(SNALF(J),J=1,NGROUP),                   *
CL    4(SNP(J),J=1,NGROUP),(SN2N(J),J=1,NGROUP),                      *
CL    5(SND(J),J=1,NGROUP),(SNT(J),J=1,NGROUP)                        *
CL    6((STRPD(J,I),J=1,NGROUP),I=1,ISTRPD)                           *
C                                                                     *
CW     (1+LTRN+LTOT+IALF+INP+IN2N+IND+INT+ISTRPD+2*IFIS+              *
CW     ICHI+(2/(ICHI+1)))*NGROUP                                      *
C                                                                     *
CB     FORMAT(4H 5D ,1P5E12.5/(6E12.5)) LENGTH OF LIST AS ABOVE       *
C                                                                     *
CD     STRPL          PL WEIGHTED TRANSPORT CROSS SECTION            *
CD                       THE FIRST ELEMENT OF ARRAY STRPL IS THE      *
CD                       CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION*
CD     STOTPL         PL WEIGHTED TOTAL CROSS SECTION                *
CD                       THE FIRST ELEMENT OF ARRAY STOTPL IS THE     *
CD                       FLUX (P0) WEIGHTED TOTAL CROSS SECTION       *
CD     SNGAM          (N,GAMMA)                                      *
CD     SFIS           (N,F)          (PRESENT IF IFIS.GT.0)          *
CD     SNUTOT         TOTAL NEUTRON YIELD/FISSION  (PRESENT IF IFIS.GT.0)*
CD     CHISO          ISOTOPE CHI  (PRESENT IF ICHI.EQ.1)            *
CD     SNALF          (N,ALPHA)    (PRESENT IF IALF.GT.0)            *
CD     SNP            (N,P)        (PRESENT IF INP.GT.0)             *
CD     SN2N           (N,2N)(LOSS) (PRESENT IF IN2N.GT.0)            *
CD     SND            (N,D)        (PRESENT IF IND.GT.0)             *
CD     SNT            (N,T)        (PRESENT IF INT.GT.0)             *
CD     STRPD          COORDINATE DIRECTION I TRANSPORT CROSS SECTION  *
CD                                  (PRESENT IF ISTRPD.GT.0)         *
C                                                                     *
C*********************************************************************
```

```
C-----------------------------------------------------------------------
CR          ISOTOPE CHI DATA                                           -
C                                                                      -
CC          PRESENT IF ICHI.GT.1                                       -
C                                                                      -
CL    ((CHIISO(K,J),K=1,ICHI),J=1,NGROUP),(ISOPEC(I),I=1,NGROUP)       -
C                                                                      -
CW    NGROUP*(ICHI+1)                                                  -
C                                                                      -
CB    FORMAT(4H 6D ,1P5E12.5/(6E12.5)) CHIISO                          -
CB    FORMAT(12I6)                     ISOPEC                          -
C                                                                      -
CD    CHIISO(K,J)   FRACTION OF NEUTRONS EMITTED IN GROUP J AS A       -
CD                     RESULT OF FISSION IN ANY GROUP USING SPECTRUM K -
CD    ISOPEC(I)     ISOPEC(I)=K IMPLIES THAT SPECTRUM K IS USED        -
CD                     TO CALCULATE EMISSION SPECTRUM FROM FISSION     -
CD                     IN GROUP I                                      -
C                                                                      -
C                                                                      -
C-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR          SCATTERING SUB-BLOCK                                       -
C                                                                      -
CC        PRESENT IF LORD(N).GT.0                                      -
C                                                                      -
CL    ((SCAT(K,L),K=1,KMAX),L=1,LORDN)                                 -
C                                                                      -
CC    KMAX=SUM OVER J OF JBAND(J) WITHIN THE J-GROUP RANGE OF THIS     -
CC       SUB-BLOCK,  IF M IS THE INDEX OF THE SUB-BLOCK, THE J-GROUP   -
CC       RANGE CONTAINED WITHIN THIS SUB-BLOCK IS                      -
CC       JL=(M-1)*((NGROUP-1)/NSBLOK+1)+1 TO JU=M*((NGROUP-1)/NSBLOK+1)-
CC    LORDN=LORD(N)                                                    -
C                                                                      -
CW    KMAX*LORDN                                                       -
C                                                                      -
CB    FORMAT(4H 7D ,1P5E12.5/(6E12.5))                                 -
C                                                                      -
CD    SCAT(K,L)     SCATTERING MATRIX OF SCATTERING ORDER L, FOR       -
CD                     REACTION TYPE IDENTIFIED BY IDSCT(N) FOR THIS   -
CD                     BLOCK,  JBAND(J) VALUES FOR SCATTERING INTO     -
CD                     GROUP J ARE STORED AT LOCATIONS K=SUM FROM 1    -
CD                     TO (J-1) OF JBAND(I) PLUS 1 TO K=1+JBAND(J),    -
CD                     THE SUM IS ZERO WHEN J=1,  J=TO=J SCATTER IS    -
CD                     THE IJJ(J)-TH ENTRY IN THE RANGE JBAND(J),      -
CD                     VALUES ARE STORED IN THE ORDER (J+JUP),         -
CD                     (J+JUP-1),...,(J+1),J,(J-1),...,(J-JDN),        -
CD                     WHERE JUP=IJJ(J)-1 AND JDN=JBAND(J)-IJJ(J)      -
C                                                                      -
C-----------------------------------------------------------------------

CEOF
```

II. BRKOXS - Bondarenko Cross-Section Data

This file is required as an adjunct to the ISOTXS file when the Bondarenko self-shielding method is to be used, Only those isotopes which have interpolation tables need be included in BRKOXS. No changes in BRKOXS-II other than the introduction of the MULT parameter are present in BRKOXS-III.

```
C*****************************************************************
C                        REVISED 07/01/73                        *
C                                                                *
CF          BRKOXS-III                                          *
CE          BONDARENKO SELF-SHIELDING TABLES                    *
C                                                                *
CN                       THIS FILE PROVIDES DATA NECESSARY FOR   *
CN                       BONDARENKO TREATMENT IN ADDITION TO     *
CN                       THOSE DATA IN FILE ISOTXS               *
CN                       FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES *
CN                       ONLY.                                   *
C                                                                *
C*****************************************************************


C----------------------------------------------------------------*
CS          FILE STRUCTURE                                      *
CS                                                              *
CS             RECORD TYPE                          PRESENT IF  *
CS             ===========================          ==========  *
CS             FILE IDENTIFICATION                  ALWAYS      *
CS             FILE CONTROL                         ALWAYS      *
CS             FILE DATA                            ALWAYS      *
CS   ************(REPEAT FROM 1 TO NISOSH)                      *
CS   *         SELF-SHIELDING FACTORS               ALWAYS      *
CS   *         CROSS SECTIONS                       ALWAYS      *
CS   *************                                              *
CS                                                              *
C                                                               *
C----------------------------------------------------------------*

C----------------------------------------------------------------*
CR          FILE IDENTIFICATION                                 *
C                                                               *
CL    HNAME,(HUSE(I),I=1,2),IVERS                               *
C                                                               *
CW    1+3*MULT                                                  *
C                                                               *
CB    FORMAT(11H 0V BRKOXS ,A6,1H*,                             *
CB   12A6,1H*,I6)                                               *
C                                                               *
CD    HNAME          HOLLERITH FILE NAME - BRKOXS - (A6)        *
CD    HUSE           HOLLERITH USER IDENTIFICATION (A6)         *
CD    IVERS          FILE VERSION NUMBER                        *
CD    MULT           DOUBLE PRECISION PARAMETER                 *
CD                       1= A6 WORD IS SINGLE WORD              *
CD                       2= A6 WORD IS DOUBLE PRECISION WORD    *
C                                                               *
C----------------------------------------------------------------*
```

```
C*****************************************************************
CR          FILE CONTROL                                          *
C                                                                 *
CL    NGROUP,NISOSH,NSIGPT,NTEMPT                                 *
C                                                                 *
CW    4                                                           *
C                                                                 *
CB    FORMAT(4H 1D ,4I6)                                          *
C                                                                 *
CD    NGROUP         NUMBER OF ENERGY GROUPS IN SET               *
CD    NISOSH         NUMBER OF ISOTOPES WITH SELF-SHIELDING FACTORS *
CD    NSIGPT         TOTAL NUMBER OF VALUES OF VARIABLE X (SEE FILE DATA*
CD                      RECORD) WHICH ARE GIVEN.  NSIGPT IS EQUAL TO *
CD                      THE SUM FROM 1 TO NISOSH OF NTABP(I)        *
CD    NTEMPT         TOTAL NUMBER OF VALUES OF VARIABLE TB (SEE FILE *
CD                      DATA RECORD) WHICH ARE GIVEN.  NTEMPT IS EQUAL *
CD                      TO THE SUM FROM 1 TO NISOSH OF NTABT(I)     *
C                                                                 *
C*****************************************************************

C*****************************************************************
CR          FILE DATA                                             *
C                                                                 *
CL    (HISONM(I),I=1,NISOSH),(X(K),K=1,NSIGPT),(TB(K),K=1,NTEMPT),  *
CL   1(EMAX(J),J=1,NGROUP),EMIN,(JBFL(I),I=1,NISOSH),             *
CL   2(JBFH(I),I=1,NISOSH),(NTABP(I),I=1,NISOSH),(NTABT(I),I=1,NISOSH) *
C                                                                 *
CW    (4+MULT)*NISOSH+NSIGPT+NTEMPT+NGROUP+1                      *
C                                                                 *
CB    FORMAT(4H 2D ,9(1X,A6)/          HISONM                     *
CB   1(18(1X,A6)))                                                *
CB    FORMAT(1P6E12.5)                 X,TB,EMAX,EMIN             *
CB    FORMAT(12I6)                     JBFL,JBFH,NTABP,NTABT      *
C                                                                 *
CD    HISONM(I)      HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6).  THESE *
CD                      LABELS MUST BE A SUBSET OF THOSE IN FILE ISOTXS *
CD                      OR GRUPXS, IN THE CORRESPONDING ARRAY.     *
CD    X              ARRAY OF LN(SIGP0)/LN(10) VALUES FOR ALL ISOTOPES, *
CD                      WHERE SIGP0 IS THE TOTAL CROSS SECTION OF THE *
CD                      OTHER ISOTOPES IN THE MIXTURE IN BARNS PER ATOM *
CD                      OF THIS ISOTOPE.  FOR ISOTOPE I, THE NTABP(I) *
CD                      VALUES OF X FOR WHICH SELF-SHIELDING FACTORS  *
CD                      ARE GIVEN ARE STORED STARTING AT LOCATION L=1+ *
CD                      SUM FROM 1 TO I-1 OF NTABP(K).             *
CD    TB             ARRAY OF TEMPERATURES (DEGREES C) FOR ALL ISOTOPES. *
CD                      FOR ISOTOPE I, THE NTBT(I) VALUES OF TB FOR *
CD                      WHICH SELF-SHIELDING FACTORS ARE GIVEN ARE  *
CD                      STORED AT LOCATION L=1+SUM FROM 1 TO I-1 OF *
CD                      NTABT(K).                                  *
CD    EMAX(J)        MAXIMUM ENERGY BOUND OF GROUP J (EV)          *
CD    EMIN           MINIMUM ENERGY BOUND OF SET (EV)              *
CD    JBFL           NUMBER OF LOWEST ENERGY GROUP FOR WHICH SELF-  *
CD                      SHIELDING FACTORS ARE GIVEN.               *
CD    JBFH           NUMBER OF HIGHEST ENERGY GROUP FOR WHICH SELF- *
CD                      SHIELDING FACTORS ARE GIVEN.               *
CD    NTABP(I)       NUMBER OF SIGP0 VALUES FOR WHICH SELF-SHIELDING *
CD                      FACTORS ARE GIVEN FOR ISOTOPE I.           *
CD    NTABT(I)       NUMBER OF TEMPERATURE VALUES FOR WHICH SELF-  *
CD                      SHIELDING FACTORS ARE GIVEN FOR ISOTOPE I.  *
C                                                                 *
C*****************************************************************
```

```
C*****************************************************************
CR          SELF-SHIELDING FACTORS                                *
C                                                                 *
CL    (((FTOT(N,K,J),N=1,NBINT),K=1,NBTEM),J=JBFLI,JBFHI),        *
CL    (((FCAP(N,K,J),N=1,NBINT),K=1,NBTEM),J=JBFLI,JBFHI),        *
CL    (((FFIS(N,K,J),N=1,NBINT),K=1,NBTEM),J=JBFLI,JBFHI),        *
CL    (((FTR (N,K,J),N=1,NBINT),K=1,NBTEM),J=JBFLI,JBFHI),        *
CL    (((FEL (N,K,J),N=1,NBINT),K=1,NBTEM),J=JBFLI,JBFHI)         *
C                                                                 *
CC    NBINT=NTABP(I)                                              *
CC    NBTEM=NTABT(I)                                              *
CC    JBFLI=JBFL(I)                                               *
CC    JBFHI=JBFH(I)                                               *
C                                                                 *
CW    5*NBINT*NBTEM*(JBFHI-JBFLI+1)                               *
C                                                                 *
CB    FORMAT(4H 3D ,1P5E12.5/(6E12.5))                            *
C                                                                 *
CD    FTOT          TOTAL SELF-SHIELDING FACTOR EVALUATED AT      *
CD                     X(N) AND TB(K).                            *
CD    FCAP          CAPTURE SELF-SHIELDING FACTOR EVALUATED AT    *
CD                     X(N) AND TB(K).                            *
CD    FFIS          FISSION SELF-SHIELDING FACTOR EVALUATED AT    *
CD                     X(N) AND TB(K).                            *
CD    FTR           TRANSPORT SELF-SHIELDING FACTOR EVALUATED AT  *
CD                     X(N) AND TB(K).                            *
CD    FEL           ELASTIC SELF-SHIELDING FACTOR EVALUATED AT    *
CD                     X(N) AND TB(K).                            *
C                                                                 *
C*****************************************************************

C*****************************************************************
CR          CROSS SECTIONS                                        *
C                                                                 *
CL    (XSPO(J),J=1,NGROUP),(XSIN(J),J=1,NGROUP),(XSE(J),J=1,NGROUP),*
CL   1(XSMU(J),J=1,NGROUP),(XSED(J),J=1,NGROUP),(XSXI(J),J=1,NGROUP)*
C                                                                 *
CW    6*NGROUP                                                    *
C                                                                 *
CB    FORMAT(4H 4D ,1P5E12.5/(6E12.5))                            *
C                                                                 *
CD    XSPO          POTENTIAL SCATTERING CROSS SECTION (BARNS)    *
CD    XSIN          INELASTIC CROSS SECTION (BARNS)               *
CD    XSE           ELASTIC CROSS SECTION (BARNS)                 *
CD    XSMU          AVERAGE COSINE OF ELASTIC SCATTERING ANGLE    *
CD    XSED          ELASTIC DOWN-SCATTERING TO ADJACENT GROUP      *
CD    XSXI          AVERAGE ELASTIC SCATTERING LETHARGY INCREMENT  *
C                                                                 *
C*****************************************************************

CEOF
```

APPENDIX I

COMPUTER CODE ABSTRACT

MINX, A MULTIGROUP INTERPRETATION OF NUCLEAR X-SECTIONS FROM ENDF/B

(1) Name of Program: MINX (Ref. 1).

(2) Computer for Which Program is Designed: CDC-6600, CDC-7600, IBM-360/91, IBM-360/195.

(3) Nature of the Physical Problem Solved: MINX calculates fine-group averaged infinitely dilute cross sections and self-shielding factors from ENDF/B-IV[1] data. Its primary purpose is to generate a pseudo-composition independent multigroup library which is input to the SPHINX[9] space-energy collapse program through standard CCCC-III[23] interfaces. MINX incorporates and improves upon the resonance capabilities of existing codes such as ETOX[5] and ENDRUN[6] and the high-order group-to-group transfer matrices of SUPERTOG[7] and ETOG.[8] Fine group energy boundaries, Legendre expansion order, gross spectral shape component (in the Bondarenko[19] flux model), temperatures and dilutions can all be used specifically.

(4) Method of Solution: Infinitely dilute, unbroadened point cross sections are obtained from resolved resonance parameters using a modified version of the RESEND program.[22] The SIGMA1[24] kernel-broadening method is used to Doppler broaden and thin the tabulated linearized pointwise cross sections at 0 K (outside of the unresolved energy region). Effective temperature-dependent self-shielded pointwise cross sections are derived from the formulation in the ETOX[5] code. The primary modification to the ETOX algorithm is associated with the numerical quadrature scheme[31] used to establish the mean values of the fluctuation intervals. The selection of energy mesh points, at which the effective cross sections are calculated, has been modified to include the energy points given in the ENDF/B file or, if the energy-independent formalism was employed, points at half-lethargy intervals. Infinitely dilute group cross sections and self-shielding factors are generated using the Bondarenko[19] flux weighting model with the gross spectral shape under user control. The integral over energy for each group is divided into a set of panels defined by the union of the grid points describing the total cross section, the reaction cross section of interest and the gross spectral shape. The integration scheme actually employed in MINX is adaptive Simpson's procedure[32] for which the initial estimate

is based on the unionized grid described above. The computation of elastic and discrete group-to-group matrices is based upon a semi-analytic scheme[18] which treats the rapidly fluctuating cross-section behavior analytically. Where this laboratory-system-based scheme becomes difficult to implement (e.g., light nuclei, inelastic thresholds), an alternative numerical integration in the center-of-mass system is employed. Multigroup transfer matrices for processes in which the outgoing neutron energy and angular distribution is uncoupled are computed by direct numerical integration.

(5) Restrictions on the Complexity of the Problem: The principal restriction is the computing time available for a given desired accuracy, number of groups, and Legendre order. The paging techniques and variable dimensioning make efficient use of available core storage; very large problems have been run with MINX (e.g., a complete 171-group P_3 neutron library at ORNL and an extensive 240-group P_4 library at LASL).

(6) Typical Machine Time (times quoted are for the CDC-7600): Typical running times are difficult to define because they are sensitive functions of the (a) accuracy required, (b) number of resonances, (c) number of groups, (d) Legendre expansion order, (e) number of temperature and dilutions, etc. Sample times are indicated below. For a problem with 50 groups, Legendre expansion P_3, generally four temperatures involving 0 K, five dilution factors, tolerances --resonance reconstruction 0.5%, linearization 0.2%, Doppler thinning 0.2%, adaptive integration 0.1%, we find:

Isotope	ENDF/B-IV Mat No.	MINX Timing (sec)
^{33}Na	1156	667
Fe	1192	1075
^{16}O	1276	590
^{238}U*	1262	6454
^{239}Pu	1264	3505

*Reconstruction tolerance 1%.

(7) Unusual Features of the Program: MINX generates and uses (in the resolved energy region) a linearly interpolable, infinitely dilute temperature-dependent pointwise cross-section library in ENDF/B-IV format.[1] This feature permits efficient computation of group cross sections with accurate Doppler broadening[24] of single-level and multilevel cross sections. The multigroup constants generated therefrom are thus known to be compatible[13] with the pointwise cross sections retrieved by continuous-energy Monte Carlo codes. New, accurate algorithms[18] for the computation of Legendre moments of group-to-group transfer matrices have been developed and implemented. These calculations are based on an expansion of the differential scattering cross section in the laboratory system and use a semi-analytic procedure which treats the rapidly fluctuating cross-section behavior analytically. Where Legendre expansion in the lab system becomes difficult (e.g., for light nuclei or near inelastic thresholds) an alternative numerical integration in the center-of-mass is employed. The procedures employed in MINX for constructing, interpolating and integrating cross sections are intended to provide and quantify user control of computational errors (assuming that the data base and weighting function are known explicitly). A paging technique[27] which manipulates huge amounts of cross-section information one block at a time (block size variable), is used throughout MINX, in addition to variable dimensioning to reduce storage requirements and to use available storage efficiently. Finally, the code and the multigroup data sets derived therefrom are intended to satisfy nuclear design standards[4] currently being implemented under auspices of the American National Standards Institute.

(8) Related and Auxiliary Programs: Three utility codes are provided to manipulate the CCCC data files.

LINX[33] -- Will combine two multi-isotope CCCC files (ISOTXS or BRKOXS only) into a new composite file in CCCC format.

BINX[33] -- Will convert CCCC data (ISOTXS, BRKOXS, or DLAYXS) from binary to BCD mode or vice-versa and selectively print the contents of the files.

CINX[34] -- Will exactly collapse fine group data (ISOTXS, BRKOXS, or DLAYXS) to a subset coarse group structure, and will also change the format of the data to 1DX/PERT-V form, if desired.

These codes were written to be as IBM-compatible as possible. The changes required are identified on the listings with "C IBM comment" cards.

(9) Status: MINX is currently operational on the CDC-7600 at Los Alamos Scientific Laboratory and the IBM 360/11 and 360/195 at Oak Ridge National Laboratory.

(10) Machine Requirements: Core and external storage such as magnetic tape or desk devices depend on the characteristics of the problem. The 50-group library would require ~330k bytes of core storage on the IBM 360 series computer or 49 000 words of SCM (no LCM) on the CDC-7600.

(11) Programming Language: MINX is coded in Standard FORTRAN-IV with data management, precision, and other features particularly adapted alternatively to CDC and IBM computers. The code is modular in structure and its output conforms to guidelines developed by the Committee on Computer Code Coordination.[11]

(12) Operating System: IBM OS 360 with the FORTRAN H compiler or LASL CROS with the CDC RUN compiler.

(13) Other Programming Information: The program consists of 227 subroutines on ~15 000 source cards. With a three-level overlay structure consisting of 11 segments, ~ 330k bytes are required on the IBM machines and $49\ 000_{10}$ words on the CDC-7600.

(14) Material Available: Source decks for MINX, LINX, BINX, and CINX can be obtained through the Argonne Code Center at ANL or the Radiation Shielding Information Center (RSIC) at ORNL. In addition, a documented report is available as part of the code package. Pointwise files have already been generated from ENDF/B-IV data and should always be used as the starting point of a MINX calculation unless specific problem application dictates otherwise. Multigroup libraries from MINX exist in 50, 126, and 171 groups. Requests for the 50-group library should be directed to the National Neutron Cross Section Center; those for the 126 and 171 libraries should be directed to RSIC.

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REFERENCES

1. M. K. Drake, "Data Formats and Procedures for the ENDF Neutron Cross Section Library," Brookhaven National Laboratory report BNL-50274 (April 1974 Revision).

2. C. R. Weisbin, P. D. Soran, D. R. Harris, R. J. LaBauve, and J. S. Hendricks, "MINX - A Multigroup Interpretation of Nuclear X-Sections," Trans. Am. Nucl. Soc., 16, 127 (1973).

3. D. R. Harris, R. J. LaBauve, R. E. MacFarlane, P. D. Soran, C. R. Weisbin, and J. E. White, "MINX, A Modular Code System for Processing Multigroup Cross Sections from Nuclear Data in ENDF/B Format," CONF-731207-1, Seminar on Codes for Nuclear Data Processing held at NEA-CPL, Ispra (December 1973).

4. "Nuclear Data Sets for Reactor Design Calculations," American National Standards Institute Standard N411, D3 (January 23, 1974).

5. R. E. Schenter, J. L. Baker, and R. B. Kidman, "ETOX, A Code to Calculate Group Constants for Nuclear Reactor Calculations," Battelle Northwest Laboratory report BNWL-1002 (ENDF-127) (1969).

6. B. A. Hutchins, C. L. Cowan, M. D. Kelley, and J. E. Turner, "ENDRUN II - A Computer Code to Generate a Generalized Multigroup Data File for ENDF/B," General Electric Co. report GEAP-13703 (ENDF-145) (March 1971).

7. R. Q. Wright, N. M. Greene, J. L. Lucius, and C. W. Craven, "SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDF/B," Oak Ridge National Laboratory report ORNL-TM-2679 (1969).

8. D. E. Kusner and R. A. Dannels, "ETOG-1, A FORTRAN IV Program to Process Data from the ENDF/B File to the MUFT, GAM, and ANISN Formats," Westinghouse Corporation report WCAP-3845-1 (ENDF-114) (December 1969).

9. N. C. Paik, W. Davis, M. B. Yarbrough, and D. Petras, "Physics Evaluations and Applications Quarterly Progress Report," Westinghouse Corporation report WARD-XS-3045-7 (1974); see also other reports in this series.

10. R. B. Kidman, R. E. Schenter, R. W. Hardie, and W. W. Little, "The Shielding Factor Method of Generating Multigroup Cross Sections for Fast Reactor Analysis," Nucl. Sci. Eng. 48, 189 (1972).

11. B. M. Carmichael, D. A. Meneley, and D. R. Vondy, "Report of the Subcommittee on Standard Interface Files, Prepared for the Committee on Computer Code Coordination," Los Alamos Scientific Laboratory report LA-5324-MS (1973).

12. C. R. Weisbin, D. R. Harris, M. E. Battat, R. J. LaBauve, W. M. Taylor, G. D. Turner, and R. E. Seamon, "Preparation of Data Libraries for Efficient Retrieval by Continuous Energy Monte Carlo Codes," Trans. Am. Nucl. Soc. 15, 572 (1972).

13. R. J. LaBauve, C. R. Weisbin, R. E. Seamon, M. E. Battat, D. R. Harris, P. G. Young, M. M. Klein, "PENDF: A Library of Nuclear Data for Monte Carlo Calculations Derived from Data in ENDF/B Format," Los Alamos Scientific Laboratory report LA-5687 (October 1974).

14. D. E. Cullen, O. Ozer, and C. R. Weisbin, "Exact Doppler Broadening of Evaluated Neutron Cross Sections," Trans. Am. Nucl. Soc. 16, 320 (1973).

15. D. R. Harris, C. B. Noll, "SUMOR (MO271), A FORTRAN-IV Program for the CDC-6600 for Neutron Resonance Cross Sections Including Level-Level Interference and Exact Doppler Broadening," Bettis Atomic Power Laboratory report WAPD-TM-810 (1969).

16. E. Oblow, "Neutron Thermalization in High Temperature Gaseous Media," thesis, Columbia University (1970).

17. E. D. Cashwell, V. R. Neergaard, N. W. Taylor, and G. D. Turner, "MCN: A Neutron Monte Carlo Code," Los Alamos Scientific Laboratory report LA-4751 (1972).

18. C. R. Weisbin, P. D. Soran, and J. S. Hendricks, "A New Procedure for the Determination of Neutron Multigroup Transfer Matrices," Nucl. Sci. Eng. 55, 329-341 (1974).

19. I. I. Bondarenko, (ed.) Group Constants for Nuclear Reactor Calculations (Consultants Bureau, New York 1964).

20. R. E. MacFarlane and M. Becker, "Self-Shielding of Elastic Transfer Matrices," Trans. Am. Nucl. Soc. 21, 495 (1975).

21. R. E. MacFarlane and M. Becker, "Self-Shielded Cross Sections for Neutron Transport in Iron," Trans. Am. Nucl. Soc. 22, 668 (1975).

22. O. Ozer, "RESEND: A Program to Preprocess EDNF/B, Materials with Resonance Files into a Pointwise Form," Brookhaven National Laboratory report BNL-17134 (1972).

23. B. M. Carmichael, "Standard Interface Files and Procedures for Reactor Physics Codes, Version III," Los Alamos Scientific Laboratory report LA-5486-MS (February 1974).

24. D. E. Cullen, "SIGMA (Version 74-1) A Program to Exactly Doppler Broaden Tabulated Cross Sections in the ENDF/B Format," Lawrence Livermore Laboratory report UCID-16426 (1974).

25. N. M. Greene, J. L. Lucius, W. E. Ford, III, J. E. White, R. Q. Wright, and L. M. Petrie, "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," Oak Ridge National Laboratory report ORNL-TM-3706 (1976).

26. J. A. Price, "A Guide to GALXY 3* Part 1," United Kingdom Atomic Energy Authority report AWRE O 40/73 (November 1973).

27. D. E. Cullen, O. Ozer, and C. R. Weisbin, "Tabular Cross Section File Generation and Utilization Techniques," Proceedings of a Conference on Nuclear Cross Sections and Technology, Vol. I, p. 419 (March 1975).

28. C. R. Lubitz, "Minutes of the Resonance Region Subcommittee," Meetings of the Cross Section Evaluation Working Group, available from National Neutron Cross Section Center (June 1974).

29. D. E. Cullen and C. R. Weisbin, "Exact Doppler Broadening of Tabulated Cross Sections," Nucl. Sci. Eng. (see preprint UCRL-76916, June 1975).

30. B. J. Toppel, A. L. Rago, and D. M. O'Shea, "MC^2, A Code to Calculate Multigroup Cross Sections," Argonne National Laboratory report ANL-7318 (1967).

31. R. N. Hwang and H. Henryson, II, "Critical Examination of Low-Order Quadratures for Statistical Integrations," Trans. Am. Nucl. Soc. 22, 712 (1975).

32. W. M. McKeeman, "Algorithm 145-Adaptive Numerical Integration by Simpson's Rule," Comm. of the Association for Computing Machinery, 5, 12 (December 1962). See also, D. Kahaner, "Comparison of Numerical Quadrature Formulas," Los Alamos Scientific Laboratory report LA-4137 (1969).

33. R. E. MacFarlane and R. B. Kidman, "LINX and BINX: CCCC Utility Codes for the MINX Multigroup Processing Code," Los Alamos Scientific Laboratory report LA-6219-MS (1976).

34. R. B. Kidman and R. E. MacFarlane, "CINX: Collapsed Interpretation of Nuclear X-Sections," Los Alamos Scientific Laboratory report LA-6287-MS (1976).

35. M. F. James, "Energy Released in Fission," J. Nucl. Energy 23, 517 (1969).

36. N. B. Gove and A. H. Wapstra, The 1971 Atomic Mass Evaluation, The Nuclear-Reaction Q-Values, (Academic Press, Inc., New York 1972).

37. C. M. Lederer, J. M. Hollander and I. Perlman, Table of Isotopes, Sixth Edition, (John Wiley and Sons, Inc., New York 1967).

38. R. B. Kidman and R. E. MacFarlane, "LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations," Los Alamos Scientific Laboratory report LA-6260-MS (1976).

39. R. E. MacFarlane and R. M. Boicourt, "NJOY: A Neutron and Photon Cross Section Processing System," Trans. Am. Nucl. Soc. 22, 702 (1975).

40. R. W. Roussin, C. R. Weisbin, J. E. White, N. M. Greene, R. Q. Wright, and J. B. Wright, "The CTR Processed Multigroup Cross Section Library for Neutronics Studies," Oak Ridge National Laboratory report ORNL-RSIC-37 (to be published).

41. C. R. Weisbin, R. W. Roussin, J. E. White, and R. Q. Wright, "Specification for Pseudo-Composition-Independent Fine-Group and Composition-Dependent-Fine and Broad-Group LMFBR Neutron-Gamma Libraries at ORNL," Oak Ridge National Laboratory report ORNL-TM-5142 (ENDF-224) (1975).

42. R. W. Hardie and W. W. Little, Jr., "1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," Battelle Northwest Laboratory report BNWL-954 (1969).

43. K. D. Lathrop, "DTF-IV, A FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," Los Alamos Scientific Laboratory report LA-3373 (1965).

44. E. M. Bohn (ed.), "Benchmark Testing of ENDF/B-IV," Brookhaven National Laboratory report ENDF-203 (1976).

45. J. E. White, R. Q. Wright, L. R. Williams, and C. R. Weisbin, "Data Testing of the 126/36 Neutron Gamma ENDF/B-IV Coupled Library for LMFRB Core and Shield Analysis," Am. Nucl. Soc. Meeting, Toronto (June 1976).

46. K. Gregson, M. F. James, and D. S. Norton, "MLBW - A Multilevel Breit-Wigner Computer Programme," United Kingdon Atomic Energy Authority report AEEW-M-517 (1965).

47. C. W. Reich and M. S. Moore, "Multilevel Formula for the Fission Process," Phys. Rev. 111, 929 (1958).

48. D. B. Adler and F. T. Adler, "Analysis of Neutron Resonances in Fissile Elements: Program CODILLI, CURVEPLOT, and SIGMA," University of Illinois at Urbana report COO-1546-3 (September 1966).

49. F. T. Adler and D. B. Adler, Proc. of Conf. on Neutron Cross Sections and Technology, Book 2, p. 873, U. S. Atomic Energy Commission Report CONF-660303 (1966).

50. E. P. Wigner and J. E. Wilkins, Jr., "Effect of the Temperature of the Moderator on the Velocity Distribution of Neutrons with Numerical Calculations for H as the Moderator," Oak Ridge National Laboratory report AECD-2275 (1944).

51. R. V. Meghreblian and D. K. Holms, Reactor Analysis, pp. 137-140, McGraw-Hill, New York (1960).

52. K. Gregson and M. F. James, "TEMPO - A General Doppler Broadening Program for Neutron Cross Sections," Atomic Energy Establishment Winfrith report AEEW-M518 (1965).

53. M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, National Bureau of Standards (1964).

54. I. A. Stegun and R. Zucker, J. Res., National Bureau of Standards report, B-Math, 74B, No. 3, 211-224 (July-September 1970).

55. G. M. Hale, D. R. Harris, and R. E. MacFarlane, "Applied Nuclear Data Research and Development Quarterly Progress Report October 1 through December 31, 1974," Los Alamos Scientific Laboratory report LA-5944-PR (April 1975), p.2.

56. O. Ozer, (ed.), "Description of ENDF/B Processing Codes and Retrieval Subroutines," Brookhaven National LAboratory report BNL-50300 (ENDF-110) (August 1971).

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