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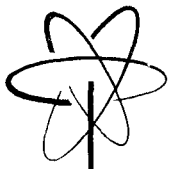

ENDRUN-II, A COMPUTER CODE TO GENERATE A GENERALIZED MULTIGROUP DATA FILE FROM ENDF/B

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GENERAL ELECTRIC

NOTICE

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ABSTRACT

1. Name: ENDRUN II
2. Computer: GE 635
3. Problem solved: ENDRUN II is used to calculate multigroup constants from energy-dependent, microscopic cross sections, resonance parameters, and inelastic level data input in the Evaluated Nuclear Data File (ENDF/B) formats. Data is processed for one material at a time and the output multigroup file includes both infinitely-dilute group cross sections and self-shielding, Bondarenko-type f-factors so that the resulting generalized file is independent of reactor composition. The multigroup data may be output on punched cards, a standard library tape, or plotted over any energy range.
4. Method of Solution: Resolved resonance parameters are evaluated according to the Doppler broadened Breit-Wigner, single-level line shape equations. Resonance contributions are averaged over each fine group with an extrapolated Romberg integration scheme. Unresolved resonance calculations employ an averaging over the χ-squared statistical distribution of resonance parameters. Self-shielding is accomplished by weighting with a $1/(\sigma_t + \sigma_o)$ flux, where σ_o is an input value representing the total other-material cross section. Provisions are made for the overlap of resolved and unresolved resonance sequences and smooth data. Separate inelastic, elastic, and n,2n matrices are calculated.
5. Restrictions on the Complexity of the Problem: ENDRUN may be used on any ENDF/B material with less than 9 isotopes. A case may include up to 100 coarse groups and 30 fine groups per coarse group. Maximum transfer matrix size is 70 x 50. Up to 5 σ_o values and 3 temperatures may be input for self-shielding.
6. Typical Running Time: A simple 29-group case for any material without resonance data is processed in only a few seconds on the GE635. A similar case for U-238 with all self-shielding options may run over an hour.

7. Unusual Features of the Program: ENDRUN is designed to allow maximum user flexibility in creating a multigroup file or testing data, e.g. several ENDF/B reactions may be combined in a single output cross section, any type of data or single cross section may be processed separately, input may come from cards, BCD or binary tape, or compressed binary tape, and matrices may be output separately or combined.
8. Related or Auxiliary Programs: ENDRUN II is a supplement to the ENDRUN I code of April, 1970 (reference 1) and retains most of the major subroutines from the earlier code. It uses several of the ENDF/B retrieval subroutines in processing the ENDF/B data file and also the QUICKW table look-up routine from MC^2. A generalized data file tape (GMUG) may be created for direct use by the TDOWN code.
9. Status: This code is in production status at GE BRDO and is executed from tape.
10. References:
1) B. A. Hutchins, L. N. Price, "ENDRUN-I, A Computer Code to Generate a Generalized Multigroup Data File from ENDF/B, GEAP-13592, April, 1970.
2) I. I. Bondarenko, Group Constants for Nuclear Reactor Calculations _ (Consultants Bureau, New York, 1964)
3) H. C. Honeck, "ENDF/B Specifications for an Evaluated Nuclear Data File for Reactor Applications", (Brookhaven, N.Y., 1966).
11. Machine Requirements: The program requires 52K memory on the GE635, including a 10K overlap with loading routines. Up to 5 tapes and 7 auxiliaries (discs at GE) may be required for some cases, but the number of tapes may be reduced by using permanent disc files and running from cards.
12. Programming Languages Used: ENDRUN is written almost entirely in FORTRAN-IV. Only those routines used in the GE compressed binary input and output options are presently written in RWSBT or NPOST languages and FORTRAN versions of these routines are also available.
13. Operating System: GECOS-III with FORTRAN-IV compiler.

14. Other Programming or Operating Information: Primary changes to convert this program to another machine would be in the input and output routines, auxiliary assignments, and particularly the plotting routines.

SECTION I

INTRODUCTION

ENDRUN was developed to provide a capability for preparing a generalized, Bondarenko-type[1], multigroup cross section file from basic nuclear data in the ENDF library format[2]. The code is a principal component of the General Electric rapid cross section adjustment technique and has been specified with a processing flexibility which allows the user to generate only a few group constants, to combine several reaction types, to punch intermediate data on cards for reuse in later computations and to specify a complete material cross section library. The code flexibility and the simplified Bondarenko approach to bypass the rigorous but expensive calculations of the neutron fluxes and system composition dependence have made ENDRUN an important tool in the LMFBR design effort.

ENDRUN II is a supplement to the ENDRUN I code of April 1970[3] and retains many of the features of the earlier code. However, some routines have been modified to improve the accuracy and/or efficiency of the computational operations. Two important modifications are:

1. The use of the Romberg integration technique for calculating the resolved resonance contribution to the coarse group cross section, and
2. The specification of a simple scattering probability function, based upon the average logarithmic energy loss, and used to generate a more explicit expression for calculating the elastic scattering transfer matrices.

The input format and computational procedures in ENDRUN II have been updated to be consistent with those formats and procedures which have been specified for the ENDF neutron cross section library of October, 1970.[4]

SECTION II

GENERAL DESCRIPTION OF ENDRUN COMPUTATIONS

The ENDRUN code generates multigroup, infinitely-dilute cross sections plus appropriate resonance self-shielding factors from pointwise data, resonance parameters and inelastic level data. The code output is used directly in TDOWN[5] to obtain effective cross sections for a specific reactor composition and flux spectrum. This output consists of the following data for a single ENDF/B material:

1. Infinitely-dilute cross sections for elastic scattering, inelastic scatter, elastic removal, fission, capture, (n,2n), and total reactions for each group of a specified multigroup structure (maximum of 100 groups).
2. Group-average values of ξ, $\bar{\mu}_{elastic}$, $\bar{\nu}$ (average neutrons emitted per fission), and χ (fission neutron fraction).
3. Downscattering matrices including elastic scattering, inelastic scattering, and (n,2n) reactions. (Maximum of 70 source and 49 downscattering groups).
4. Resonance self-shielding factors for up to 3 material temperatures and 5 values of σ_o (parameter specifying total cross section per atom of resonance material). These self-shielding factors are to be used together with the infinitely-dilute cross sections for elastic scattering, fission, capture, and total reactions to obtain effective group constants, as well as to compute the contribution this material makes to σ_o, when computing self-shielding for other materials (maximum of 100 groups with self-shielding).

The calculation of groupwise cross sections is carried out by flux-weighting the data in the ENDF/B libraries and is based upon three broad categories of data - resolved resonance parameters, unresolved resonance parameters and smooth pointwise cross section values. The resonance contributions to the groupwise cross sections are computed with the Breit-Wigner single-level formula and are combined with the smooth values which contribute to a specified energy range. Any degree of overlapping of smooth data, resolved resonance energy ranges and unresolved resonance energy ranges is permitted, with the resonance contributions summed over all isotopes. Secondary energy distributions may be used along with smooth data to compute the scattering matrices. The forms taken by the secondary energy distributions are limited to discrete energy loss, Maxwellian distributions and tabulated data for both the inelastic scattering and the (n,2n) reactions. The reaction parameters, ξ and $\bar{\mu}_{elastic}$, are averaged by weighting with the product of the flux and elastic cross section, while $\bar{\nu}$ is weighted with the product of flux and fission cross section. The values of χ are determined from the secondary energy distributions for fission neutrons and are limited to Maxwellian distributions, simple fission distributions and the Watt fission spectrum.

Self-shielding factors are calculated by computing groupwise self-shielding cross sections for each combination of temperature and σ_o and dividing by the infinitely-dilute value. The smooth data, as well as the resonance contributions to the cross sections, may be self-shielded, with the smooth self-shielding being temperature independent and the resonance contribution computed for each temperature. The resolved resonance pointwise cross sections are obtained by summing the contribution from all important resolved resonances, each described by the appropriate Doppler-broadened, Breit-Wigner single-level line shape, including potential scattering interference. Contributions from unresolved resonances include first order corrections for overlapping of resonances from the same and different sequences. Averaging over chi-squared distributions of the fission and scattering widths is accomplished by dividing the distributions into either 5 or 10 equally probable portions, depending upon the number of degrees of freedom in the distribution, and using representative values

of the widths in each portion. Distributions with 5 or more degrees of freedom are taken to be delta functions. Average resonance widths may be specified as a function of energy in ENDF/B. Both the resolved and unresolved resonance contributions can be computed for s, p and d waves, with up to 5 J states, each, depending on the number of isotopes and ranges.

Flux weighted, average cross sections are obtained by averaging over energy groups, subgroups and points. The structure of the groups and the application of the groups and points are summarized as follows:

1. Coarse Groups - group structure which is specified by the user for the output multigroup cross section file. The number of coarse groups must not exceed 100.

2. Fine Groups - basic subdivision of the coarse groups which is used directly to average all non-resonance data and for the final averaging of all resonance cross sections. Up to thirty fine groups may be specified for each coarse group.

3. Ultra-fine Groups - subdivisions of the fine groups which are used only for the numerical integration of resolved and unresolved resonances. The number of ultra-fine groups in the resolved resonance energy range is computed by the code based upon a convergence criterion for the Romberg integration method. The ultra-fine groups in the unresolved resonance energy range are determined from the resonance width, the Doppler width and the distance from the resonance peak. Integration of unresolved resonances is carried out by using Simpson's rule.

4. Unresolved Integration Points - energy points used for the integration over single representative resonances in the unresolved resonance averaging procedure. The contribution from all resonances is determined at the specified energy and subsequent averaging is carried out by interpolation to the fine groups and flux weighting to obtain the coarse group values.

The fluxes which are used for weighting factors in the averaging procedures are expressed as the product of a coarse variation and a fine variation in the neutron flux,

$$\phi(E) = F(E)C(E)$$

The fine variation, F(E), results in the resonance self-shielding and is based on the constant collision density (narrow resonance) approximation which gives

$$F(E) \propto \frac{1}{\Sigma_t(E)}$$

$$\propto \frac{1}{\sigma_{t,m}(E) + \sigma_o}$$

where $\sigma_{t,m}(E)$ is the energy dependent, total cross section of the material and σ_o is the self-shielding, other material, input parameter. The coarse flux variation, C(E), may be input by the user. However, in the more general case, the coarse flux will be represented in the code by the fission neutron spectrum at high energies and by the inverse energy below an input break-point.

An elastic removal cross section for the coarse group is computed as

$$\sigma_{er} = \frac{\xi\sigma_{es}}{\Delta u}$$

using the group average values of ξ and σ_{es}. Thus, the elastic removal cross section is independent of a particular flux distribution (except for the implied 1/E flux representation)and must be corrected in the later application of the TDOWN code (Reference 5).

A complete problem in ENDRUN (that is, for a material containing resolved and unresolved resonance data as well as smooth data and for a relatively large number of coarse groups) may require extensive computations. Therefore, provisions for partial computations have been made. Averaging may be limited to any specified number of sequential coarse

groups of a given group structure, in which case only the cross sections contributing to the specified groups are considered (including the contributions from resolved resonances outside the specified groups), and all transfer terms out of the specified groups in the scattering matrices are computed. To avoid repeating lengthy computations of the pointwise resonance cross sections, intermediate data values may be punched on cards for use at a later time. Partial computations may be performed by limiting the reaction types considered or by computing only infinitely-dilute cross sections, infinitely-dilute cross sections with self-shielding factors, or infinitely-dilute cross sections with scattering matrices. These options for partial calculations give the user the flexibility needed to update existing coarse-group files without recomputing all coarse group data for a given material. Thus, file updating may be accomplished in a relatively simple manner where changes are made in ENDF/B data over limited energy ranges, in one or two types of data (smooth, resolved or unresolved resonance, or secondary energy distributions), or in one or two of the reaction types.

Input to ENDRUN allows the user many options in addition to those described above. The reaction types from the ENDF/B file which are to be included in each of the reaction types on the coarse group file are specified by the user (e.g., the coarse group capture cross section may include the (n,γ), (n,α) and (n,p) reactions from ENDF/B). Data in the ENDF/B format may be overlaid by card input. The coarse groups in which smooth data contribute to the self-shielding factors are specified by the user. (The user must have a good knowledge of the ENDF/B data being used.) The self-overlap correction for unresolved resonances is limited to energies above a given input value. The energy range over which unresolved resonances contribute is specified (normally corresponding to the ENDF/B data), and unresolved contributions to the self-shielding factors are considered only below a given energy. The contributions of resolved resonances to both the infinitely-dilute cross sections and the self-shielding factors is indicated by coarse groups.

ENDRUN output includes coarse group data both printed and on tape for use with the TDOWN code. In addition, coarse group infinitely-dilute cross sections, self-shielding factors and scattering matrices may be plotted as functions of neutron energy.

SECTION III

DETAILED DESCRIPTION OF ENDRUN COMPUTATIONS

3.1 Averaging Techniques

The methods for processing the ENDF/B data are based upon averaging techniques which use a flux weighting over fine and ultra-fine subdivisions of the coarse group energy structure. The averaging techniques vary with the type of data that is being processed and with the type of output that is being requested. An understanding of the averaging procedures is necessary to the understanding of the code formulation in the remainder of this section.

3.1.1 Energy Group Structure

The coarse group energy structure is input by the user and is divided into a specified number of equal lethargy width fine groups. The fine group is the basic unit for processing data in ENDRUN and up to thirty such groups may be specified for each coarse group. The actual number of fine groups to be used is dependent upon the importance of the energy range and the degree of fluctuation in the data.

Fine groups are used directly in the averaging of smooth, pointwise cross sections and reaction parameters. However, the fine groups must be further subdivided to evaluate the resolved and unresolved resonances.

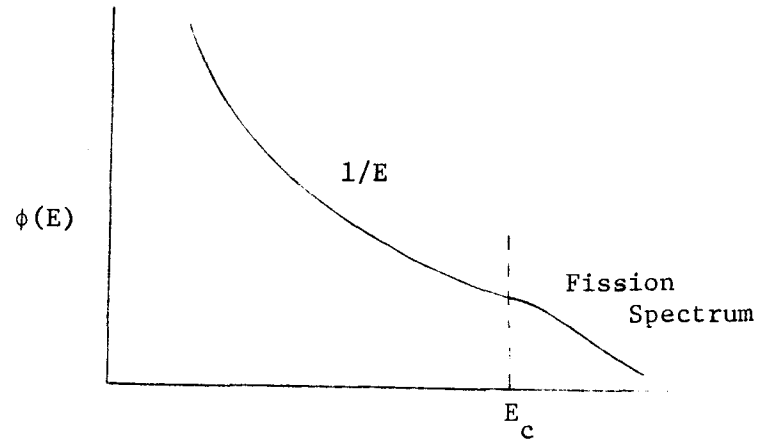
The cross sections for the resolved resonance energy range are calculated by the Romberg numerical integration technique over ultra-fine energy groups (see Section 3.2). The number of ultra-fine groups is computed by the code (initially one ultra-fine group per fine group) and is doubled in successive Romberg calculations until the fine group values satisfy a

specified convergence criterion. A maximum of 2^8 ultra-fine groups is permitted by the code but this value may be overlaid by the user.

Designated energy points are used for the integration over single representative resonances in the unresolved resonance averaging procedure. Integration is carried out by using Simpson's rule over ultra-fine groups which are determined by the resonance width, the Doppler width and the distance from the resonance peak (see Section 3.3). The result of these integrations is a point cross section value for a given energy and temperature, averaged over the distribution of resonance parameters.

3.1.2 Neutron Flux Spectra for Cross Section Averaging

Reaction rates for each material are preserved during a multigroup averaging procedure by weighting the fine and ultra-fine group cross sections with their respective fine and ultra-fine group neutron flux. This flux spectrum over energy is actually spatially and composition dependent. However, the multigroup approach assumes that such dependencies have a very small effect on the average cross section value if the coarse group lethargy width is small and flux does not change radically. Accordingly, the flux weighting used in ENDRUN is assumed to be the product of a fine flux which may vary radically with energy and a coarse flux which does not. The fine flux, taken as $1/\sigma_t$, is calculated separately within each averaging procedure. The coarse flux is assumed to vary as the fission spectrum above a specified cutoff energy, E_c, and to vary inversely with the energy below the cutoff value. The coarse flux representation is calculated only once for each fine group and later used in all averaging procedures.



The flux shape must be continuous across the boundary between the two spectra (see sketch). This is accomplished by the following normalization:

$$\phi(E) = 1/E = \sqrt{\frac{E}{T^3}}\; e^{-E/T} \quad \text{at } E = E_c \tag{1.1}$$

$$\text{normalization factor } \phi_N = E_c\sqrt{\frac{E_c}{T^3}}\; e^{-E_c/T} = 1 \tag{1.2}$$

$$\text{normalized } \phi(E) = \frac{\phi(E)}{\phi_N} = \frac{\sqrt{\frac{E}{T^3}}\; e^{-E/T}}{\sqrt{\frac{E_c}{T^3}}\; e^{-E_c/T}} = \frac{E}{E_c^3}\, e^{\frac{E_c - E}{T}} \tag{1.3}$$

Since most of the integrations performed in ENDRUN involve a $\phi(E)dE$ term, it is this product which is actually calculated and called the "fine group flux", ϕ_j. The above expression for the fission spectrum is unfortunately not directly integrable, but can be evaluated at the fine group average energy, E_{av}, and multiplied by the energy width of the group. In the equations below, E_j is the fine group, mid-lethargy energy, Δu_j is the fine group lethargy width, and ΔE_j is the fine group energy width.

<u>1/E Region</u>

$$\phi_j = \int_{E_L}^{E_U} \frac{1}{E}\, dE = \Delta u_j \tag{1.4}$$

Fission Spectrum

$$\phi_j = \int_{E_L}^{E_U} \sqrt{\frac{E}{E_c^3}}\, e^{(E_c-E)/T}\, dE \simeq \sqrt{\frac{E_{av}}{E_c^3}}\, e^{(E_c-E)/T}\, \Delta E_j \qquad 1.5$$

where $E_L = E_j\, e^{-\Delta u_j/2}$, lower energy

$E_U = E_j\, e^{\Delta u_j/2}$, upper energy

$E_{av} = \frac{E_L + E_U}{2}$

$\Delta E_j = E_U - E_L$

Since the cutoff energy, E_c, is a completely arbitrary input parameter, the group in which E_c falls is a special case:

$$\phi_j = \int_{E_L}^{E_C} \frac{1}{E}\, dE + \int_{E_C}^{E_U} \sqrt{\frac{E}{E_c^3}}\, e^{(E_c-E)/T}\, dE \qquad 1.6$$

$$\simeq \left[\Delta u_j - \log \frac{E_U}{E_c}\right] + \left[\sqrt{\frac{E_{av}}{E_c^3}}\, e^{(E_c - E_{av})/T}\, \Delta E_j\right] \qquad 1.7$$

where $E_{av} = \frac{E_c + E_U}{2}$

$\Delta E_j = E_U - E_c$

The flux representation described above is expected to be adequate for the generation of most multigroup cross section sets. However, a more descriptive spectra may be input for each coarse group and used as interpolation points for determining the fine group fluxes. The input fluxes are assumed to be pointwise values per unit lethargy.

3.1.3 Averaging of Smooth, Pointwise Data

Smooth cross sections and reaction parameters are given in File 3 of ENDF/B for specified energy points. These energy points are not necessarily the same for all reactions and the interpolation mode may also vary - even for the same reaction type. The interpolation mode will be either linear, semi-log or log-log and will be used to generate the fine group cross sections and reaction parameters at the mid-lethargy energy points of the fine group. Several input reaction types may be combined into one output reaction by interpolating each data array separately and summing the fine group values. It should be noted that a zero interpolation will result if an energy point is either above or below the given range.

The smooth data is directly averaged for those coarse groups outside the resolved resonance energy range. Within the resolved range, smooth data for the fine groups is added to the contributions from the resolved resonances before obtaining the coarse group values. Combinations of those contributions from smooth data, unresolved resonances and resolved resonances include an adjustment in the self-shielding cross sections (a first order overlap correction) for the value of the self-shielding parameter, σ_o.

3.1.4 Infinitely Dilute Cross Section Averaging

The assumption of infinite dilution implies that there is so little of the material in specified region that the material has no effect upon the flux (i.e., the fine flux $(1/\sigma_t)$ is assumed to be constant). Whether or not this is ever a realistic approximation, the concept is useful because self-shielding f-factors can later be applied to the infinitely dilute cross section values to account for variation in the fine flux.

The infinitely-dilute, coarse group average for reaction x over group I is given by:

$$\left\langle \sigma_x^{\infty} \right\rangle_I = \frac{\int_{E_L}^{E_U} \sigma_x(E)\,\phi(E)\,dE}{\int_{E_L}^{E_U} \phi(E)\,dE} \qquad 1.8$$

In performing this integration in ENDRUN, it is assumed that the coarse group can be broken into enough fine groups, j, to allow a replacement of the integral by a summation. In effect, this implies that all sharp resonances are given with resonance parameters in ENDF/B file 2, not as smooth pointwise data in file 3. The significance of "sharp" will obviously vary with the size of the coarse group. A 0.25 lethargy width divided into 25 fine groups per coarse group at 1 keV provides a point separation of 1 eV. A larger group width or fewer fine groups would be more restrictive.

Assuming this spacing is adequate, the interpolated cross section values, σ_{x_j}, and calculated fine group flux, ϕ_j, may be used to rewrite the average as:

$$\left\langle \sigma_x^{\infty} \right\rangle_I = \frac{\sum \sigma_{x_j}\,\phi_j}{\sum \phi_j} \qquad 1.9$$

This basic expression is used throughout ENDRUN. Only the method of determining the fine group σ_{x_j} varies with the type of data.

3.1.5 Self-Shielded Cross Section Averaging

A cross section is said to be self-shielded if enough of the material is present to change the flux acting upon it. The amount of change will depend on the total cross section at each point which in turn is the sum of the total cross section of the material itself and the total "other-material" cross section. In practice this latter value will depend on the specific reactor composition, but the Bondarenko f-factor method approximates the specific case and facilitates the creation of a general file by calculating self-shielded cross sections for only certain specified values of other-material total cross section, σ_o, which are assumed to be constant over energy. In later design calculations, the actual value of σ_o for a material, m, is calculated for each energy group by taking:

$$\sigma_o^m = \frac{\sum_{n \neq m} N^n \sigma_t^n}{N^m}$$

and the self-shielding factors are interpolated to this value (see Reference 5).

The self-shielded, coarse group average for reaction x over group I for an "other-material" cross section σ_o is given by:

$$\left\langle \sigma_x(\sigma_o) \right\rangle_I = \frac{\int_{E_L}^{E_U} \frac{\sigma_x(E)}{\sigma_t(E) + \sigma_o} \phi(E)dE}{\int_{E_L}^{E_U} \frac{1}{\sigma_t(E) + \sigma_o} \phi(E)dE} \qquad 1.10$$

where $\phi(E)$ is the slowly varying flux described in Section 3.1.2. The material index, m, has been dropped for convenience.

Equation 1.10 can be rewritten as a summation by assuming, as in Section 3.1.4, a slowly varying cross section. Thus,

$$\left\langle \sigma_x(\sigma_o) \right\rangle_I = \frac{\sum \frac{\sigma_{x_j} \phi_j}{\sigma_{t_j} + \sigma_o}}{\sum \frac{\phi_j}{\sigma_{t_j} + \sigma_o}} \qquad 1.11$$

Once the fine group cross sections, σ_{x_j} and σ_{t_j}, have been determined, the self-shielded weighting may be rapidly performed for several σ_o values.

While the above equations will hold for any standard reaction - capture, elastic or inelastic scattering, capture, n_2n, etc. - they do not provide the correct weighting to conserve transport reaction rates according to the diffusion equation. A separate treatment is therefore necessary for the transport cross section, σ_t.

3.1.6 Special Averaging for the Transport Cross Section

Energy averaging of the transport cross section over coarse group I is accomplished by flux-weighting the mean free path, λ_{tr},

$$\left\langle \lambda_{tr} \right\rangle_I = \frac{\int_{E_L}^{E_U} \lambda_{tr}(E)\phi(E)\, dE}{\int_{E_L}^{E_U} \phi(E) dE} \qquad 1.12$$

With the relationship $\Sigma_{tr}(E) = 1/\lambda_{tr}(E)$, the average macroscopic transport cross section, $\left\langle \Sigma_{tr} \right\rangle$, is given by:

$$\langle \Sigma_{tr} \rangle_I = \frac{\int_{E_L}^{E_U} \phi(E)dE}{\int_{E_L}^{E_U} \frac{\phi(E)\,dE}{\Sigma_{tr}(E)}} \qquad 1.13$$

Over the energy range of interest, the greatest contribution to Σ_{tr} comes from Σ_t. Hence, the average total cross section is given by:

$$\langle \Sigma_t \rangle_I = \frac{\int_{E_L}^{E_U} \phi(E)dE}{\int_{E_L}^{E_U} \frac{\phi(E)dE}{\Sigma_t(E)}} \qquad 1.14$$

Applying the narrow resonance approximation and multiplying the numerator and denominator of the upper integral by $\Sigma_t(E)$, this becomes:

$$\langle \Sigma_t \rangle_I = \frac{\int_{E_L}^{E_U} \frac{\Sigma_t(E)\,dE}{\left[\Sigma_t(E)\right]^2}}{\int_{E_L}^{E_U} \frac{dE}{\left[\Sigma_t(E)\right]^2}} \qquad 1.15$$

If m is a material index, then for a particular composition,

$$\Sigma_t(E) = \sum_m N^m \sigma_t^m(E) \qquad 1.16$$

where: $\sigma_t^m(E)$ is the microscopic total cross section of material m. Defining $\langle \Sigma_t \rangle$ by a similar expansion over composition and noting the definition of σ_o^m, the microscopic averaging of σ_t (again dropping the index m) is accomplished by:

$$\langle \sigma_t \rangle_I = \frac{\int_{E_L}^{E_U} \frac{\sigma_t(E)dE}{[\sigma_t(E) + \sigma_o]^2}}{\int_{E_L}^{E_U} \frac{dE}{[\sigma_t(E) + \sigma_o]^2}} \qquad 1.17$$

3.2 Resolved Resonances

Resolved resonance calculations are carried out in ENDRUN by evaluating each resonance, as defined by ENDF/B file 2 parameters, according to the single-level Breit-Wigner formula, including scattering interference. If a resonance contributes more than a specified amount to any cross section at the upper or lower energies of a coarse group, it is integrated -- by an extrapolated Romberg technique[6] -- over each fine group within that coarse group. The resolved resonance contribution is calculated at as many points (equally spaced over the lethargy range of the fine group) as are necessary to achieve a sufficient accuracy in the average fine group cross section value. The contributions from all resonances are summed and added to the appropriate smooth data. The fine group cross sections are then averaged using the narrow resonance approximation to obtain coarse group average cross sections. Self-shielded cross sections are calculated for several values of σ_o and temperature and are corrected for the overlap of unresolved and resolved sequences. The specific capabilities are:

1) Up to 50 coarse groups may have resolved resonance contributions.
2) Up to 30 fine groups per coarse group.
3) Up to 8 isotopes per material.
4) Up to 7 resonance ranges per isotope.
5) Up to 5 σ_o values per calculation.
6) Up to 3 temperatures per calculation.

Optional intermediate output from the resolved resonance calculation includes both fine and coarse group averages for smooth plus resolved contributions to the total, scattering, capture, and fission cross sections. Both infinitely-dilute and self-shielded values are output.

3.2.1 Basic Theory and Assumptions

The coarse group average cross section for reaction type x and group I is defined as:

$$\langle \sigma_x \rangle_I = \frac{\int_{E_L}^{E_U} \phi(E)\sigma_x(E)dE}{\int_{E_L}^{E_U} \phi(E)dE} \qquad 2.1$$

where E_L and E_U are the lower and upper energy bounds of the coarse group.* To evaluate Equation 2.1 over the resolved resonance energy range, the following assumptions are made:

1) The resonance cross section is described by the Doppler-broadened, Breit-Wigner, single-level formula.
2) All resonances are assumed to be narrow with respect to the average energy loss per collision with any nuclei.
3) There is no appreciable resonance overlap due to other materials.
4) The contribution to the total cross section from all other isotopes can be represented by the input constant σ_o.

The formulae appearing in Gregson, et al.,[7] omitting the interference scattering term, have been adopted in the data formats and procedures manual for the ENDF neutron cross section library (Reference 4) and are used to specify the cross section value at energy E for reaction type x due to resonance r as follows:

Scattering

$$\sigma_{n,r} = \frac{\pi}{k^2} g_j \left[\frac{\Gamma_{n,r}\cos 2\phi_\ell - 2\Gamma_{n,r}\Gamma_{\gamma r}\sin^2\phi_\ell + 2(E-E'_{o,r})\Gamma_{n,r}\sin 2\phi_\ell}{(E-E'_{o,r})^2 + \left(\frac{\Gamma_r}{2}\right)^2} \right] \qquad 2.2a$$

*For the treatment of the transport cross section see Section 3.1.6.

Capture and fission

$$\sigma_{x,r} = \pi/k^2 \; g_j \; \frac{\Gamma_{n,r}\,\Gamma_{x,r}}{(E-E_{o,r})^2 + \left(\frac{\Gamma_r}{2}\right)^2} \qquad 2.2b$$

where k = neutron wave number

$$= 2.19685 \left(\frac{A}{A+1.0}\right) \times 10^{-3} \sqrt{E}$$

g_j = statistical spin factor for resonance r = $\frac{2j+1}{2(2I+1)}$

A = atomic weight of target nucleus

I = spin of target nucleus

j = spin of the compound nucleus for resonance r

ℓ = angular momentum state of incident neutron for resonance r

ϕ_ℓ = phase shift

$= ka'$ for $\ell = 0$

$= ka' - \tan^{-1}(ka')$ for $\ell = 1$

$= ka' - \tan^{-1}(3ka'/(3-(ka')^2))$ for $\ell = 2$

a' = effective scattering radius (in units of 10^{-12} cm)

$E'_{o,r}$ = the effective resonance energy

$$= E_{o,r} + \frac{S_\ell(|E_{o,r}|) - S_\ell(E)}{2P_\ell(|E_{o,r}|)} \; \Gamma_{n,r}(|E_{o,r}|)$$

$E_{o,r}$ = the energy at the resonance peak

S_ℓ = the shift factor

$= 0$ for $\ell=0$

$= 1/(1+ka)$ for $\ell=1$

$= -(18+3(ka)^2)/(9+3(ka)^2 + (ka)^4)$ for $\ell=2$

P_ℓ = the penetration factor

$= ka$ for $\ell=0$

$= (ka)^3/(1+ka)^2)$ for $\ell=1$

$= (ka)^3/(9+3(ka)^2 +(ka)^4$ for $\ell=2$

a = channel radius (in units of 10^{-12} cm)

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

and $\Gamma_{x,r}$ is the partial width of reaction type x in resonance r. The capture and fission partial widths are assumed to be independent of the incident neutron energy. However, the scattering and total widths vary with energy as follows:

$$\Gamma_{n,r}(E) = \frac{P_\ell(E)\ \Gamma_{n,r}(|E_{o,r}|)}{P_\ell(|E_{o,r}|)} \qquad 2.3$$

and

$$\Gamma_r(E) = \Gamma_{n,r}(E) + \Gamma_{\gamma,r} + \Gamma_{f,r} \qquad 2.4$$

where the absolute value of the resonance energy is used for bound levels.

A potential scattering cross section corresponding to the effective hard sphere scattering is also included in the scattering and total cross section. The potential scattering term is determined from

$$\sigma_{pot}(E) = \sum_\ell (2\ell+1)\frac{4\pi}{k^2}\ \sin^2\phi_\ell \qquad 2.5$$

where the summation is over all angular momentum states.

The reaction cross sections for a specific energy E' includes the contribution from each resonance and the appropriate potential scattering term as follows:

Scattering

$$\sigma_n(E') = \sum_r \sigma_{n,r}(E') + \sigma_{pot}(E') \qquad 2.6$$

Capture and Fission

$$\sigma_x(E') = \sum_r \sigma_{x,r}(E') \qquad 2.7$$

Total

$$\sigma_T(E') = \sigma_n(E') + \sigma_\gamma(E') + \sigma_f(E') \qquad 2.8$$

Equations 2.2 through 2.8 apply to a system in which the target nucleus is essentially at rest with respect to the neutron motion. At elevated temperatures, the nuclear thermal motion is significant and the right hand side of the Equations 2.2a and 2.2b must be replaced with averages over the nuclear velocities. Assuming a Maxwellian velocity distribution for the nuclei and neglecting the resonance energy dependence of those parameters which are slowly varying functions of energy (e.g., Γ_n, Γ_t, ϕ_ℓ and k), the temperature dependent cross sections become[8]

Scattering

$$\sigma_{s,r}(E) = \sigma_{o,r}\left[\frac{\Gamma_{n,r}}{\Gamma_{t,r}}\cos 2\phi_\ell - \frac{\Gamma_{\gamma,r}}{\Gamma_{t,r}} 2\sin^2\phi_\ell\right]\psi(\chi,\xi) + \frac{\sigma_{o,r}}{2}\sin 2\phi_\ell\ \chi(\chi,\xi) \qquad 2.9$$

Capture and Fission

$$\sigma_{x,r}(E) = \sigma_{o,r}\frac{\Gamma_{x,r}}{\Gamma_{t,r}}\psi(\chi,\xi) \qquad 2.10$$

where $\sigma_{o,r} = \frac{4\pi}{k^2} gj \frac{\Gamma_{n,r}}{\Gamma_{t,r}}$

$\xi = \Gamma_{t,r}/\Delta$

Δ = Doppler width $= \sqrt{\frac{4E_{o,r}k'T}{A}}$

T = material temperature in °K

$$\chi = 2/\Gamma_{t,r} (E' - E_{o,r})$$

k'= Boltzman constant

$$y = 2/\Gamma_{t,r} (E - E_{o,r})$$

$\psi(\chi,\xi)$ = the Doppler broadened Breit-Wigner, line shape function

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

and

$\chi(\chi,\xi)$ = the Doppler broadened interference line shape function

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

The values of $\psi(\chi,\xi)$ and $\chi(\chi,\xi)$ are found by using the QUICKW table look-up subroutine of previously-calculated values.[9]

The energy-dependent neutron flux in Equation 2.1 is based upon the gross spectrum and local flux variations, as discussed in Section 3.1.2, and is expressed as

$$\phi(E) = \frac{\phi_c(E)}{\sigma_T(E) + \sigma_o} \qquad 2.11$$

where $\sigma_T(E)$ = total cross section

σ_o = the total cross section per atom of material due to all other materials (an input constant)

$\phi_c(E)$ = Coarse flux representation which varies inversely with energy unless specified in the input.

The total cross section in Equation 2.11 should include all contributions from the material itself (resolved resonance, unresolved resonance and smooth) in order to give the correct self-shielding effects. This is accomplished by summing the infinitely dilute total cross section contributions over all resonances and all isotopes and then adding in the smooth contribution which was calculated earlier. The only contribution not included is thus from the unresolved resonance range. A standard correction can be made to the resolved resonance self-shielded cross sections to account for an overlap of the resolved and unresolved energy range, but for the case in which the complete unresolved energy range ends in the same coarse group that the resolved range starts, a more accurate method is used. In this case, the fine group average values of the unresolved total cross section are carried into the resolved link and explicitly included in $\sigma_T(E)$ of Equation 2.11. The details of the overlap calculation and correction factors are given in Section 3.5.

3.2.2 Numerical Integration Method

Equation 2.1 is evaluated over the fine group by using the Romberg numerical integration scheme (Reference 6). Thus,

$$\int_{u_L^{fine}}^{u_U^{fine}} f(u)du = \lim R_{2^{K_N}}^{(K)} \qquad 2\text{-}12$$

where $f(u)^+$ = separate independent evaluation for both the numerator and denominator of Equation 2.1.

$$R_{2^{K_N}}^{(m)} = \left(4^m R_{2^{K_N}}^{(m-1)} - R_{2^{(K-1)}N}^{(m-1)}\right) \Big/ \left(4^m - 1\right)$$

$$m = 1, 2 \text{---------} K$$

+Note that lethargy and energy are used interchangeably. f(u) is actually evaluated at the energy endpoints of the ultra-fine subdivision of the fine groups.

$R_{2^{K_N}}^{(o)}$ = Trapezoidal-rule approximation to the integral calculated from the subdivision of the fine group lethargy range into 2^{K_N} equal parts

$= w\,[1/2\, f(u_0) + f(u_1) + \text{-----} f(u_{2^{K_N}-1}) + 1/2\, f(u_{2^{K_N}})]$

w = subdivision lethargy width

$= (u_U^{fine} - u_L^{fine})/2^{K_N}$

u_U^{fine} = Upper lethargy of the fine group

u_L^{fine} = Lower lethargy of the fine group

$u_0 = u_L^{fine}$

$u_{2^{K_N}} = u_u^{fine}$

$u_1 = u_0 + w$, etc.

$N = 2^{\ell}$, where the trapezoidal approximation using 2^{ℓ} subdivisions is within 10% of the trapezoidal approximation using $2^{\ell+1}$ subdivisions.

The approximation is sufficiently accurate when

$$\left| R_{2^{(K-1)_N}} - R_{2^{K_N}} \right| \Big/ R_{2^{K_N}} \leq \varepsilon \qquad 2\text{-}13$$

where ε is set at 0.001, but may be altered in the input.

3.3 UNRESOLVED RESONANCES

Unresolved resonance parameters are given in File 2 of ENDF/B for use in the Breit-Wigner single-level formula with interference. The data for each material, isotope and energy range can be read according to three options which are available for specifying the average properties of the resonances. The options are:

1. Resonance parameters are given for each ℓ and j state and are independent of energy.
2. Resonance parameters, with the exception of the average fission width, are given for each ℓ and j state and are independent of energy - fission widths are tabulated for specified energies.
3. Resonance parameters for each ℓ and j state are tabulated as a function of specified energy points.

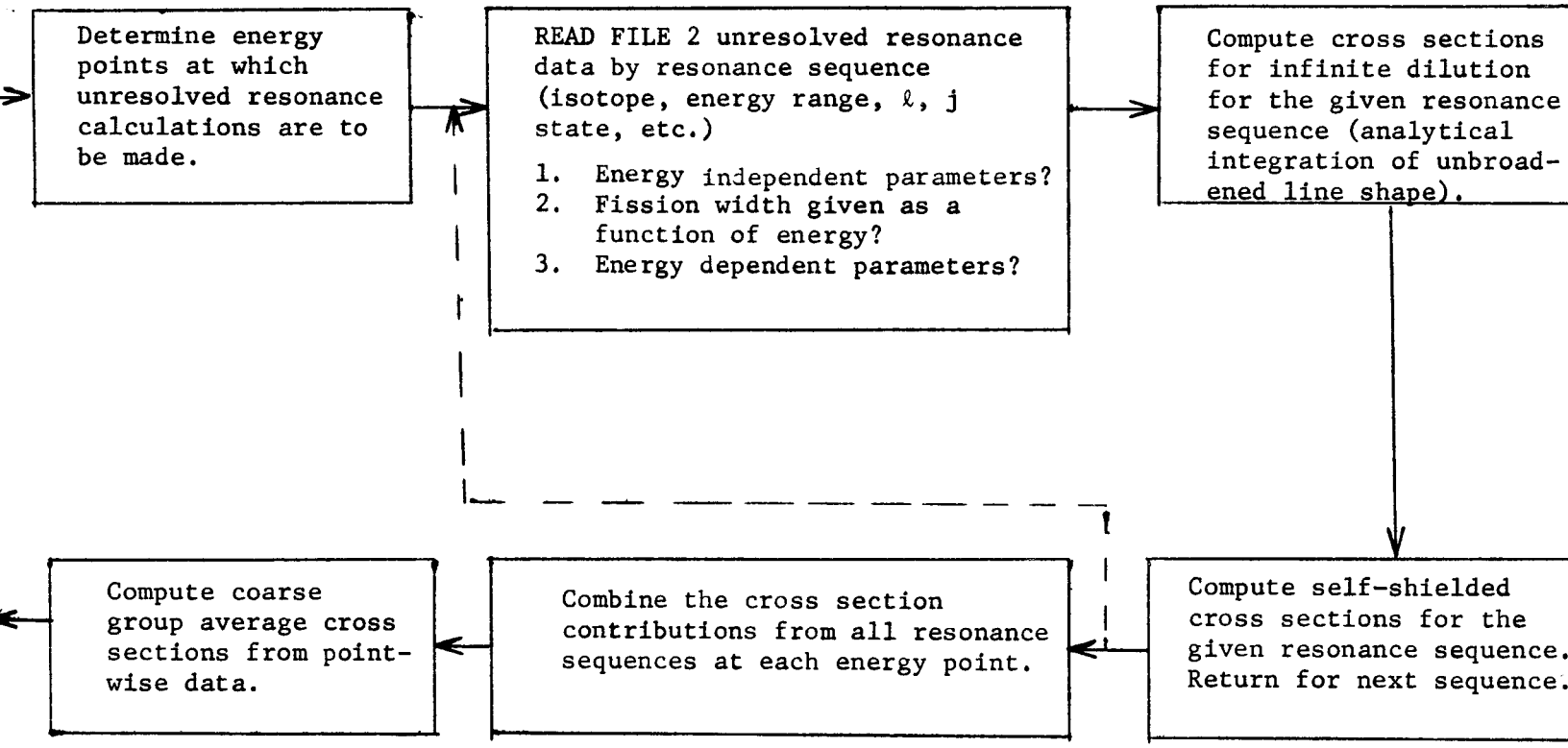
ENDRUN will handle data for up to 8 isotopes, 7 energy ranges, 15 (ℓ,j) states, and 30 energy points for a single material.

A generalized flow diagram for the unresolved resonance calculation is shown in Figure IV.1. The computation of the coarse group average cross section begins with the calculation of average infinitely dilute and self-shielded cross sections at specified energy points across the total unresolved energy range. The endpoints of this range are the input quantities URR(1) and URR(3), and should normally correspond to the low and high extremes of all the unresolved resonance energy ranges of all isotopes. The energy points are arbitrarily selected and need not coincide with the energy points given in ENDF/B. Infinitely dilute cross sections are computed for (n,f), (n,γ), (n,n) and (n,t) reactions at each energy point, while corresponding self-shielded cross sections for each value of σ_o and temperature are computed only at those points which do not exceed the input energy URR(2). Since the self-shielded computation may be time consuming, the pointwise cross sections may be optionally punched on cards and used in subsequent problems for that material.

Following the generation of all the pointwise cross sections, coarse group values are computed by interpolation and averaging over fine groups.

FIGURE IV.1

GENERALIZED FLOW DIAGRAM OF UNRESOLVED RESONANCE CALCULATIONS



These coarse group cross sections are later combined with contributions from the resolved resonances and smooth data to form the complete set of cross sections for the coarse groups. Special treatment is given for the single coarse group which contains the lower energy bound of the unresolved resonance range. For this group, unresolved contributions to σ_t are computed and saved in the fine group structure so that they may be later used directly in the self-shielding calculations for the combined resolved and smooth contributions. The manner in which the resolved and unresolved overlap calculations are carried out is described in Section 4.4.

3.3.1 Resonance Sequences

The pointwise infinitely-dilute and self-shielded cross sections are computed independently for each combination of (ℓ,j) state, energy group and isotope. These independently computed cross sections are then combined according to the appropriate isotopic abundances by a) adding the infinitely-dilute cross sections which apply at each point, and b) using a routine which applies a first order correction to self-shielded cross sections to account for the contribution of each to the total cross section seen by the others (see Section 3.4). Since each resonance sequence, which is defined by the combined (ℓ,j) state, energy range, and isotope,is independent of the others, the first-order correction can be made by considering only the average cross sections, (i.e. after the integrations over single resonances are completed). If $\sigma_{x,c}(\sigma_o,T)$ is the cross section for reaction x, sequence c, and specific values of σ_o and T, the combined cross section at energy point E is given by

$$\sigma_x^E(\sigma_o,T) = \sum_{\text{all } c} B_c \, \sigma_{x,c}^E(\sigma_o',T) \qquad 3.1$$

where

$$\sigma_o' = \sigma_o + \sum_{c'\neq c} B_{c'} \, \sigma_{t,c'}^E(\sigma_o,T) \qquad 3.2$$

and B_c = relative abundance for the isotope of sequence c.

Values of $\sigma^E_{x,c}(\sigma'_o,T)$ are obtained from the $\sigma^E_{x,c}(\sigma_o,T)$ values by a Taylor expansion. This correction is in the direction of unself-shielding the cross sections for a given σ_o and is primarily important for small values of σ_o.

Since the independent resonance sequences are defined by (ℓ,j) state, energy range and isotope, contributions from a given sequence are computed only at those energy points which fall within that particular range. Thus there is no restriction placed on the limits of the energy ranges, and ranges of different sizes, with any degree of overlapping, can be considered. However, the limits of the ranges will not be strictly honored since interpolation between points is performed. For example, when an unresolved range ends between consecutive unresolved energy points, the contribution from that range will be felt throughout the interval between the points by way of interpolation. Also, of course, the input energies URR(1) and URR(3) define the absolute limits of the unresolved resonance contributions regardless of the ranges on ENDF/B. Any ranges or parts of ranges which fall outside of these limits are simply ignored.

3.3.2 Treatment of Statistical Distributions of Resonance Parameters

The pointwise cross sections for each sequence are obtained by averaging over χ^2 distributions for the fission and neutron widths. These distributions are approximated by the use of discrete values for the parameters, each representing an equal portion of the distribution. Ten values of the discrete parameters are used for distributions with 1 and 2 degrees of freedom, five values for 3 and 4 degrees of freedom and the single average value when there are 5 or more degrees of freedom. The discrete parameters are computed from the average parameters by use of the multiplying factors, g_x, given in Table B.1. That is,

$$\Gamma_x = g_x \langle \Gamma \rangle$$

for either the fission or neutron width. The values of g_x used here are those generated for the MC^2 code (reference 9).

TABLE 3.1

MULTIPLYING FACTORS FOR OBTAINING DISCRETE PARAMETERS

TO REPRESENT χ-SQUARED DISTRIBUTIONS

		g_x				
x	for ν =	1	2	3	4	5
1		.005254	.051755	.189269	.254966	1.0
2		.037174	.163089	.476304	.549072	
3		.103133	.288398	.793185	.842565	
4		.207850	.431720	1.23576	1.23075	
5		.359875	.599144	2.30575	2.12265	
6		.574320	.800477			
7		.879486	1.05263			
8		1.33502	1.39297			
9		2.10558	1.91582			
10		4.39230	3.30400			

3.3.3 Pointwise Cross Section Generation for a Given Sequence

Cross sections are computed from the Breit-Wigner line shape formula with interference and the computations are consistent with those procedures described for the ENDF neutron cross section library (reference 4). Analytical integration is carried out for the infinitely-dilute calculation, resulting in the following simple recipes:

Scattering

$$(\sigma^{E}_{n,c})^{\infty} = \left(\frac{2\pi^2}{k^2}\right)\left(\frac{g_c}{D_c}\right)\left[\frac{\langle\Gamma_n\rangle^{E}_{c}\ \langle\Gamma_n\rangle^{E}_{c}}{\langle\Gamma_T\rangle^{E}_{c}} S^{E}_{n,c} - 2\,\bar{\Gamma}^{E}_{n,c}\sin^2\phi_\ell\right] \qquad 3.3$$

Capture and Fission

$$(\sigma^{E}_{x,c})^{\infty}_{x=n} = \left(\frac{2\pi^2}{k^2}\right)\left(\frac{g_c}{D_c}\right)\frac{\langle\Gamma_n\rangle^{E}_{c}\ \langle\Gamma_x\rangle^{E}_{c}}{\langle\Gamma_T\rangle^{E}_{c}} S^{E}_{x,c} \qquad 3.4$$

where $(\sigma^{E}_{x,c})^{\infty}$ = infinitely-dilute cross section for reaction x, sequence c at energy E.

k = neutron wave number

$$= 2.19685\ \left(\frac{A}{A+1.0}\right) \times 10^{-3}\ \sqrt{E}$$

g_c = statistical spin factor for sequence c = $\frac{2j+1}{2(2I+1)}$

D_c = average level spacing for sequence c

ϕ_ℓ = phase shift

$= ka'$ for $\ell=0$

$= ka' - \tan^{-1}(ka')$ for $\ell=1$

$= ka' - \tan^{-1}\left(\frac{3ka'}{3-(ka')^2}\right)$ for $\ell=2$

A = atomic weight of the target nucleus

I = spin of the target nucleus

a' = effective scattering radius (in units of 10^{-12}cm)

and $\langle \Gamma_n \rangle_c^E$, $\langle \Gamma_x \rangle_c^E$ and $\langle \Gamma_T \rangle_c^E$ are the partial widths for sequence c at energy E for scattering, reaction x and total respectively. The factor $S_{x,c}^E$ corrects for the parameter distribution and is given by

$$S_{x,c}^E = \frac{\left\langle \frac{\Gamma_{n,c}^E \Gamma_{x,c}^E}{\Gamma_{T,c}^E} \right\rangle}{\frac{\langle \Gamma_n \rangle_c^E \langle \Gamma_x \rangle_c^E}{\langle \Gamma_T \rangle_c^E}} \qquad 3.5$$

Equation 3.5 is numerically evaluated by using discrete parameters derived from the factors given in Table 3.1.

The potential scattering cross section, $\sigma_{p,c}$, associated with the particular sequence c, is added to the resonance contribution. It is computed as follows:

$$\sigma_{p,c} = \frac{4\Pi}{k^2} g_c \nu_c \sin^2 \phi_\ell \qquad 3.6$$

where ν_c is the number of degrees of freedom for the neutron width and the remaining terms are described above. Because of the energy dependence of the neutron wave number, k, and the phase shift, ϕ_ℓ, a potential scattering contribution is calculated at each resonance energy.

The average neutron width in equations 3.3, 3.4 and 3.5, $\langle \Gamma_n \rangle_c^E$, is obtained from the reduced neutron width, $\langle \Gamma_n^o \rangle_c^E$, by taking

$$\langle \Gamma_n \rangle_c^E = \langle \Gamma_n^o \rangle_c^E \nu_c V_\ell \sqrt{E} \qquad 3.7$$

where V_ℓ = penetration factor for the given ℓ state

$= 1$ for $\ell = 0$

$= (ka)^2/(1+(ka)^2)$ for $\ell = 1$

$= (ka)^4/(9+3(ka)^2+(ka)^4)$ for $\ell = 2$

and a = the penetration shift radius = $[1.23(A)^{1/3} + 0.8] \times 10^{-1}$

Self-shielded cross sections are derived from Doppler-broadened, Breit-Wigner, single-level line shapes. In this case, integration over single resonances is done numerically, with the self-shielding based on the narrow-resonance approximation. Thus, for a given energy point and sequence,

$$\sigma_{x,c}^{E}(\sigma_o,T) = \frac{\sum_{i}^{I}\sum_{m}^{M}\int_{E}^{\infty}\frac{\sigma_{x,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')}{\sigma_o+\sigma_{t,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')+\sigma_{p,c}}dE'}{\sum_{i}^{I}\sum_{m}^{M}\int_{E}^{E+D_c/2}\frac{dE'}{\sigma_o+\sigma_{t,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')+\sigma_{p,c}}} \qquad 3.8$$

where the summations are over the discrete parameters representing the distributions, and integration is necessary over only one side of the resonance since the contribution from interference terms is neglected. It is assumed that the resonance spacing is constant at D_c. Thus, to obtain an energy-averaged cross section, the integration in the denominator is terminated at half the resonance spacing. Other quantities in Equation 3.8 are:

$\sigma_{x,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')$ = Breit-Wigner, energy dependent cross section for reaction x; discrete parameters $\Gamma_{f,i}$, $\Gamma_{n,m}$, and temperature T.

$\sigma_{p,c}$ = potential scattering cross section from Equation 3.6 associated with resonance sequence c.

The Doppler-broadened, energy-dependent cross section in Equation 3.8 is computed as follows:

Scattering

$$\sigma_{n,c}(\Gamma_{f,i},\Gamma_{n,m},T,E') = \left[\frac{4\pi g_c}{k^2}\left[\left(\frac{\Gamma_n\Gamma_n}{\Gamma_T}\right) - 2\Gamma_n \sin^2\phi_\ell\right]\right] \psi(T,E) \qquad 3.9$$

Capture and Fission

$$\sigma_{x,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')_{x\neq n} = \frac{4\pi g_c}{k^2}\left(\frac{\Gamma_n\Gamma_x}{\Gamma_T}\right)\psi(T,E) \qquad 3.10$$

where the values of Γ_n, Γ_x and Γ_T correspond to the discrete parameters for the specific i, m values in Equation 3.8 and k is the neutron ware number at the specified resonance energy for sequence c. The form of the Breit-Wigner line shape, $\psi(T,E')$, is the same as that given for the resolved resonance calculation (Section 3.2.1) and is obtained from the table of the complex probability function W, with

$$\psi(\xi,\chi) = \frac{\xi\sqrt{\pi}}{2}\ \mathrm{ReW}\left(\frac{\xi\chi}{2}\ ,\ \frac{\xi}{2}\right), \qquad 3.11$$

using the QUICKW Routine (reference 9).

Integration over energy (reduced variable χ) is carried out by using Simpson's rule in four ranges containing different step sizes. For $\xi \geq 1.0$, integration is carried out to $\chi = 375.6$, and for $\xi < 1.0$, it is terminated at $\chi = 375.6/\xi$. For fission, capture and elastic scattering reactions, the following remainder term is added:

$$R = \frac{1}{\sqrt{\beta(1+\beta)}}\left(\frac{\pi}{2} - \arctan\chi\sqrt{\frac{\beta}{1+\beta}}\right) \qquad 3.12$$

with

$$\beta = \frac{\sigma_o + \sigma_{p,c}}{\sigma_{x,c}(\Gamma_{f,k},\ \Gamma_{n,\ell},T,E)}$$

$$\chi = 375.6.$$

For the total cross section, the remainder is given by

$$R_t = R/(\sigma_o + \sigma_{p,c}) \qquad 3.13$$

The values of $\sigma_{p,c}$, Γ_n for different ℓ states, and energy dependent partial widths are obtained in the same manner as for the infinitely-dilute cross

sections. For the total cross section, Equation 3.8 is modified to use weighting by the square of the denominator under the integral signs, as described in Section 4.1.6.

Several options are available for the evaluation of Equation 3.8 (see the input entry description for LFLUXC). It is recommended that the RAPTURE option[10] be used since the other techniques are for special situations and can give erroneous results if used incorrectly. The RAPTURE procedure is based upon the following approximation over the interval from E to E + $D_c/2$.

$$\sigma_{t,c}^{BR}(\Gamma_{f,i}\,\Gamma_{n,m},T,E') << \sigma_o + \sigma_{p,c}$$

Equation 3.8 then becomes

$$\sigma_{x,c}^{E}(\sigma_o,T) = \frac{2(\sigma_o+\sigma_{p,c})}{D_c I M}\sum_{i}^{I}\sum_{m}^{M}\frac{\sigma_{x,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')\,dE'}{\sigma_o+\sigma_{t,c}(\Gamma_{f,i},\Gamma_{n,m},T,E')+\sigma_{p,c}} \qquad 3.14$$

A self-overlap correction, based on Nicholson's Method A[11], can be applied as a first order correction to the RAPTURE approximation in cases where the resonances are broad compared to the spacing. The following formula is used for this correction:

$$\sigma_{x,c}^{E,F}(\sigma_o,T) = \sigma_{x,c}^{E,IN}(\sigma_o,T) + \frac{e}{E_x}\left[(\sigma_{x,c}^{E})^{\infty} - \sigma_{x,c}^{E,IN}(\sigma_o,T)\right] \qquad 3.15$$

with the superscripts IN and F referring to initial and final (corrected) cross sections. The value of E_x depends upon the distribution of resonance widths and is given by

$$E_x = \frac{\left\langle \frac{\Gamma_n^2\,\Gamma_x}{\Gamma_t} \right\rangle}{\left\langle \Gamma_n \right\rangle \left\langle \frac{\Gamma_n \Gamma_x}{\Gamma_t} \right\rangle} \qquad 3.16$$

where the averages are obtained by using the discrete values described in Section 3.3.2, Treatment of Statistical Distributions of Resonance Parameters. The value of e is dependent on the distribution of level spacings and is

approximated by taking

$$e = 1.6\ y\ G(y) \qquad 3.17$$

where $G(y) = 1 - \sqrt{\pi}\ y\ \exp(y)\ \mathrm{erfc}\ (y^{\frac{1}{2}})$.

and $y = \xi^2/4$

This expression for e is based on a $\nu = 10$ chi-squared distribution for the resonance spacing. In ENDRUN, e is approximated by

$$e = 1.0 - 0.62\ y^{-0.3} \qquad 3.18$$

The effect of the self-overlap correction is to bring the cross section which was computed using the RAPTURE approximation closer to the infinitely-dilute value.

Since the self-shielded cross sections are numerically integrated over each representative resonance while an analytically integrated form is used for the infinitely-dilute cross sections, there will be small differences between the results. These differences are eliminated by performing a numerical integration with $\sigma_o = 10^{12}$ and normalizing to the previously computed infinitely dilute value. This normalization is performed for each resonance sequence.

The use of the generalized parameter σ_o for the self-shielding computations eliminates the need to account for resonance heterogeneity effects in the ENDRUN code. Heterogeneity effects may be considered in the TDOWN code (reference 5) or other codes which use the generalized file by applying a correction factor to the homogeneous σ_o value. Since it is assumed that composition effects on self-shielding can be satisfactorily computed by use of this single, generalized parameter, it is unnecessary to consider in ENDRUN the factors which go into generating this parameter for real cases.

3.4 TRANSFER MATRICES

Downscattering matrices in the coarse group structure can be computed for inelastic scattering, elastic scattering and the (n,2n) reaction. These cross sections may be output separately in the generalized file format or can be combined into a single transfer matrix.

3.4.1 Inelastic Scattering

The inelastic scattering reaction is characterized by a physical process in which the subject nucleus is first excited to a higher energy state by an incident neutron of energy E and then de-excited by emitting a neutron of energy E'. The secondary energy distribution of the "scattered" neutron may be described by either an excitation energy, Q, for a particular level in the residual nucleus or by an effective nuclear temperature, θ, for the continuum reaction. Both reaction types may be included for a given material.

Pointwise cross sections and reaction Q-values (excitation energies) are given in File 3 of ENDF/B for the excited levels. Partial transfer cross sections from coarse group I to coarse group M, due only to the level data, are computed as follows:

$$\sigma_{in}^{level}(I \to M) = \frac{\sum_{k=1}^{N} \sum_{j} \sigma_{in,j,k}\, \phi_j\, \delta_{k,j}}{\sum_{j} \phi_j} \qquad 4.1$$

where k = index of a discrete level (N levels)

j = fine group index

$\sum_{j}$ = Summation over all fine groups in coarse group I

$\sigma_{in,j,k}$ = inelastic cross section for level k interpolated to the mid lethargy energy of fine group j

ϕ_j = fine group flux

$\delta_{k,j}$ = 1 if $E_{L,M} \leq E' = (E + Q_k)^{+} < E_{U,m}$

= 0 otherwise

$E_{U,m}$ = Upper energy in group M

$E_{L,M}$ = lower energy in group M

+ The excitation energies are given as negative values.

The continuum contribution to the transfer matrix is determined from a normalized probability distribution, $P(E \rightarrow E')$ and can be broken down into partial energy distributions, $f_k(E \rightarrow E')$, where each of the partial distributions can be described by different analytic representations.

$$P(E \rightarrow E') = \sum_{k=1}^{K^{max}} P_k(E) f_k(E \rightarrow E') \qquad 4.2$$

and at a particular incident neutron energy, E,

$$\sum_{k=1}^{K^{max}} P_k(E) = 1 \qquad 4.3$$

where $P_k(E)$ is the fractional probability that the distribution $f_k(E \rightarrow E')$ can be used at incident energy E. The probability and distribution functions are given in File 5 of ENDF/B.

An integrated distribution function is defined as

$$F_k(j \rightarrow M) = \int_{E'_{L,M}}^{E'_{U,m}} f(E_j \rightarrow E')dE' \qquad 4.4$$

where j = represents a fine energy group

M = coarse group M

E_j = the mid lethargy energy of fine group j

$E_{U,m}$ = upper energy of coarse group M

$E_{L,M}$ = lower energy of coarse group M

Finally, partial transfer cross sections from coarse group I to coarse group M, due to the continuum, are computed as follows:

$$\sigma_{in}^{cont}(I\to M) = \frac{\sum_{k=1}^{N}\sum_{j}\sigma_{in,k,j}\,P_{k,j}\,\phi_j\,F_k(j\to M)}{\sum_{j}\phi_j} \qquad 4.5$$

where j, k, $\sum_{j}$, $\sigma_{in,j,k}$, ϕ_j, $E_{U,m}$, $E_{L,M}$ are defined as in

Equation 4.1

$P_{k,j}$ = the fractional probability of the mid-lethargy energy of fine group j

$F_k(j\to M)$ is represented by various analytical formulations based upon an identification number (LF number) from the ENDF/B library. Only LF=3 and 9 are presently available for specifying the distribution function in ENDRUN.

LF = 3 Excitation of discrete levels+

$$F_k(j\to M) = \int_{E_{L,M}}^{E_{U,m}} \delta\left[E' - \frac{A^2+1}{(A+1)^2}E + \frac{A}{A+1}\phi_j\right] dE'$$

= 1 if $E_{L,M} \le E' < E_{U,m}$ and E' satisfies the conditional delta function equality

= 0 otherwise

ϕ_j = excitation energy of the residual nucleus at the mid-lethargy energy of fine group j

+ This distribution function is presently available but would not normally be used to describe a continuum reaction.

LF = 9 Maxwellian distribution

$$F_k(j\to M) = \int_{E_{L,M}}^{E_{U,m}} \frac{E'}{I}\, e^{-E'/\phi_j}\, dE'$$

$$= \phi_j^2 \left[e^{-E_{L,M}/\phi_j} (E_{L,M}/\phi_j + 1) - e^{-E_{U,m}/\phi_j} (E_{U,m}/\phi_j + 1) \right]$$

I = normalization constant

$$= \phi_j^2 \left[1 - e^{-(E_j - u_j)/\phi_j} \left(1 + \frac{E_j - U_{k,j}}{\phi_j} \right) \right]$$

ϕ_j = nuclear temperature at the mid-lethargy energy of fine group j

$U_{k,j}$ = a constant to define the upper limit for the final neutron energy for partial reaction k such that

$$0 \le E' \le E_j - U_{k,j}$$

The transfer cross sections are determined by adding together the partial contributions,

$$\sigma_{in}(I\to M) = \sigma_{in}^{\text{level}}(I\to M) + \sigma_{in}^{\text{cont}}(I\to M) \qquad 4.6$$

and normalizing the sum of the matrix terms to the total inelastic scattering for group I, given by,

$$\sigma_{in,I} = \frac{\sum_{k=1}^{N} \sum_{j} \sigma_{in,k,j}\, \phi_j}{\sum_{j} \phi_j} \qquad 4.7$$

where all the terms have been defined for Equation 4.1 except that N corresponds to the total level and continuum partial contributions to the inelastic cross section.

For the case in which the sum of the matrix terms is less than the total inelastic cross section, as for a truncated matrix, the difference is added to the last matrix term (i.e., added to the lowest downscattering transfer cross section). For the case in which the sum of the matrix terms is larger than the total inelastic cross section, each matrix term is reduced in proportion to its magnitude.

3.4.2 (n,2n) and (n,3n) Reactions

The (n,2n) and inelastic reactions are similar processes and the (n,2n) downscattering terms are calculated as in Equation 4.5 with $\sigma_{in,k,j}$ replaced by $\sigma_{(n,2n),k,j}$ (the k^{th} partial level or continuum (n,2n) cross section evaluated at the mid-lethargy energy of fine group j). The distribution functions for determining the normalized probability distributions of the (n,2n) reaction are limited to the same analytical formulations as specified for the inelastic reaction. Namely, the excitation of discrete levels and the Maxwellian distributions. The distributions are also limited, by the ENDF/B format, to those cases in which the exit neutrons have the same energy.

The sum of the (n,2n) matrix terms is normalized to twice the total (n,2n) cross section for group I to account for the production of two neutrons. That is

$$\sum_{m=1}^{I^{max}} \sigma_{n,2n}^{(I\rightarrow M)} = 2\sigma_{(n,2n),I} \qquad 4.8$$

The (n,3n) reaction is handled in the same manner as the (n,2n) reaction and is added to the (n,2n) matrix. For this case, the sum of the matrix terms is set equal to three times the coarse group average cross section prior to being added to the (n,2n) matrix and the average (n,3n) cross section, $\sigma_{(n,3n),I}$ is added to $\sigma_{(n,2n),I}$.

3.4.3 Elastic Scattering

The transfer cross sections due to elastic scattering are calculated by two different methods depending upon the lethargy group width and the magnitude of the average logarithmic energy loss. If the logarithmic energy loss for coarse group I, ξ_I, is "small" as compared to the lethargy width for either coarse group I or I+1, then Method 1 is used. For ξ_I "large" as compared to the coarse group widths, Method 2 is used. (Note that ξ_I is a previously calculated quantity - see Section 3.5.1). The criteria for determining whether ξ_I is small is based upon the input parameter, F_ξ, and the following inequalities,

$$\xi_I \leq F_\xi (\Delta u)_I \qquad 4.9$$

$$\xi_I \leq F_\xi (\Delta u)_{I+1} \qquad 4.10$$

where Δu is the lethargy width for the coarse group. ξ_I is considered small if both inequalities are satisfied.

Method 1 - ξ_I small as compared to $(\Delta u)_I$ and $(\Delta u)_{I+1}$

The elastic removal expression for coarse group I is calculated as follows:

$$\sigma_{er_I} = b_I \, \xi_I \, \sigma_{S_I} / \Delta u_I \qquad 4.11$$

where σ_{S_I} = scattering cross section for group I which has been previously calculated from resolved, unresolved and smooth data.

b_I = a correction factor to be calculated

and ξ_I and $(\Delta u)_I$ are defined above.

Equation 4.11, without the b_I term, is the familiar expression for scattering out of group I in a 1/E flux spectrum. The b_I term is then a correction factor to account for a flux shape which is other than a 1/E distribution.

When coarse group input fluxes have not been specified, b_I will be dependent upon the input cut-off energy, E_c, which is used to distinguish between the 1/E flux variation and the fission spectrum flux representation (see Section 3.1.2). Thus, for lethargies greater than u_c (corresponding to the cut-off energy), b_I will be equal to 1. That is,for

$$u_I - 2/3\ \xi_I \geq u_c \qquad 4.12$$

For lethargies less than the cut-off lethargy, b_I will be determined for a fission spectrum flux shape and given as,

$$b_I = \left(\frac{(\Delta u)_I}{\phi_I}\right)\left(\frac{E_{\xi_I}}{E_c}\right)^{3/2} \exp\left(\frac{-10^6(E_{\xi_I} - E_c)}{\theta}\right) \qquad 4.13$$

where E_{ξ_I} = energy corresponding to the average lethargy for coarse Group I = $10^7 \exp(-\mu_I + 2/3\xi_I)$

θ = fission spectrum temperature

ϕ_I = summation over the fine group fluxes = $\sum_j \phi_j$

and the remaining terms are defined above.

When coarse group fluxes have been input and used to calculate the fine group fluxes, b_I is given by

$$b_I = \Delta u_I/\phi_I \qquad 4.14$$

It is recognized that this type of correction will present special problems in codes which process the generalized file output from ENDRUN and attempt to correct the elastic removal cross section for the true flux spectrum representation. These correction techniques are discussed in TDOWN (reference 5).

The transfer matrix for elastic scattering is not calculated since the assumption that ξ_I is small compared to $(\Delta u)_{I+1}$ implies that the transfer will only be from one group to the next. Thus, the transfer cross section will be equal to the elastic removal.

Method 2 - ξ_I large as compared to $(\Delta u)_I$ and $(\Delta u)_{I+1}$

The second method for calculating downscattering cross sections is based upon a simple probability function for scattering from lethargy u to lethargy u'. This probability function for coarse group I is given as follows

$$P_I(u \to u') = A_I(u'-u) + B_I \qquad 4.15$$

where $u_{U,I} \geq u \geq u_{L,I}$ and A_I and B_I are group constants which are determined from the solution of simultaneous equations for the average logarithmic energy loss, ξ_I, and the scattering probability normalized over all lethargies. That is,

$$\int_u^{u+\ell n\frac{1}{\alpha}} P(u \to u')du' = \int_u^{u+\ell n\frac{1}{\alpha}} \left[A_I(u'-u)+B_I\right] du' = 1 \qquad 4.16$$

and

$$\int_u^{u+\ell n\frac{1}{\alpha}} (u'-u)P(u \to u')du' = \int_u^{u+\ell n\frac{1}{\alpha}} \left[A_I(u'-u)^2 + B_I(u'-u)\right] du' = \xi_I \qquad 4.17$$

here $\ell n\frac{1}{\alpha}$ is the maximum lethargy gain for scattering from the target nucleus and α has the usual meaning, $\alpha = \left(\frac{A-1}{A+1}\right)^2$.

The simultaneous solution of Equations 4.10 and 4.11 gives for A_I and B_I,

$$A_I = \frac{\xi_I - \frac{1}{2}\ell n\frac{1}{\alpha}}{\frac{1}{12}\ell n^3\frac{1}{\alpha}} \qquad 4.18$$

$$B_I = \frac{\frac{1}{3}\ell n\frac{1}{\alpha} - \xi_I/2}{\frac{1}{12}\ell n^2\frac{1}{\alpha}} \qquad 4.19$$

The probability for scattering from a fine group j within coarse group I, to above an arbitrary lethargy u_k is next determined from the expression,

$$P(j \rightarrow u > u_k) = \int_{u_{U,j}-\alpha'\Delta u_j}^{u_{U,j}} du \int_{u_k}^{u+\ell n\frac{1}{\alpha}} P(u \rightarrow u')du' \qquad 4.20$$

where $u_{L,j}$ = lower lethargy of fine group j

$u_{U,j}$ = upper lethargy of fine group j

$u_{U,I}$ = upper lethargy for coarse group I

Δu_j = lethargy width of fine group j

α' = fraction of the fine group j lethargy width which can scatter neutrons above lethargy u_k

$= 1$ for $(u_k - \ell n\frac{1}{\alpha}) \leq u_{L,j}$

$= \dfrac{u_{U,j} - (u_k - \ell n\frac{1}{\alpha})}{\Delta u_j}$ for $u_{U,j} > (u_k - \ell n\frac{1}{\alpha}) > u_{L,j}$

$= 0$ for $u_{U,j} \leq (u_k - \ell n\frac{1}{\alpha})$

Substituting Equation 4.15 into Equation 4.20 and carrying out the integration gives

$$P(j \rightarrow u > u_k) = \frac{A_I}{2} \alpha'\Delta u_j \left[(B_I/A_I + \ell n\tfrac{1}{\alpha})^2 - (u_k - u_{U,j} + B_I/A_I)(u_k - u_{U,j} + \alpha'\Delta u_j + B_I/A_I) + \frac{\alpha'^2 \Delta u_j^2}{3} \right] \qquad 4.21$$

For the case in which $u_k = u_{U,I}$, Equation 4.21 gives the probability for scattering from coarse group I. Thus, the elastic removal cross section is given the following expression,

$$\sigma_{er,I} = \frac{\sum_j \sigma_{s_I} P(j \to u > u_{U,I}) \phi_j}{\sum_j \phi_j} \qquad 4.22$$

where the summation is over all fine groups j in coarse group I.

The downscattering terms from coarse group I to coarse group M are calculated in a manner similar to Equation 4.22. That is,

$$\sigma_{er}(I\ M) = \frac{\sum_j s_j (P(j \to u > u_{L,M}) - P(j \to u > u_{U,m}))\phi_j}{\sum_j \phi_j} \qquad 4.23$$

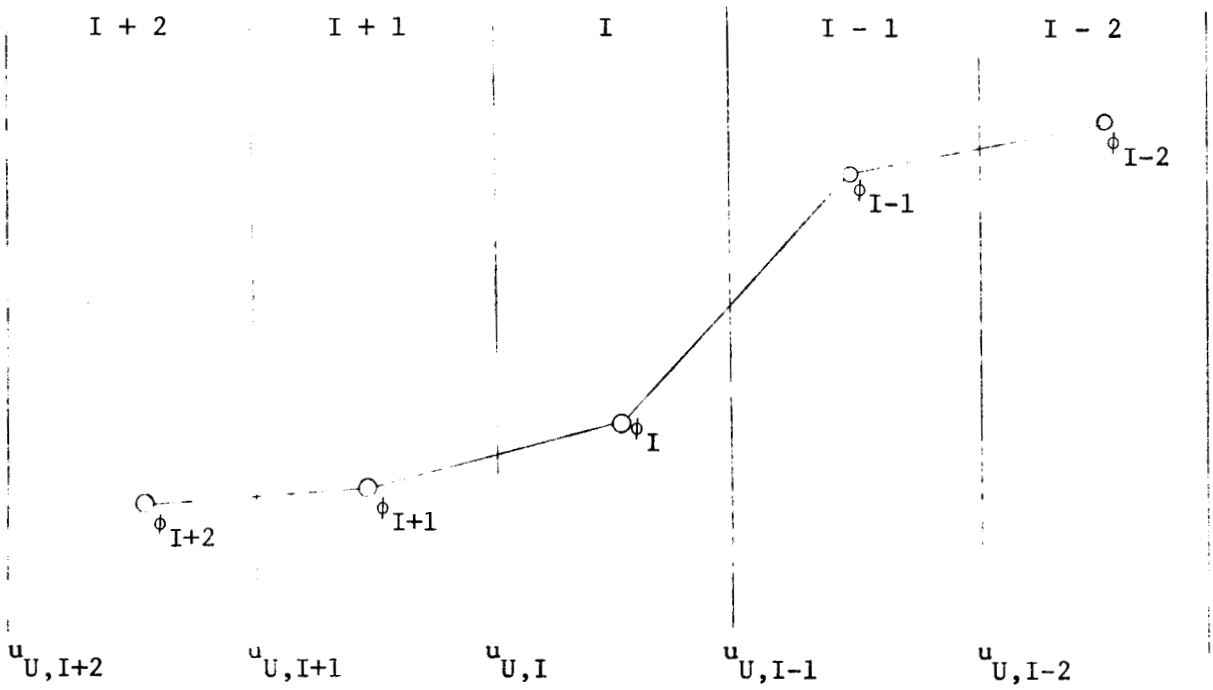
where $P(j \to u > u_{U,m}) = 0$ if neutrons are not scattered into coarse group M+1.

3.4.4 Lethargy Gain Indicator

A lethargy gain indicator is included in the ENDRUN output for each coarse group I and is identified as follows:

Indicator	Condition
1	$\ell n \frac{1}{\alpha} \leq \frac{\Delta u_I}{2}$
2	$\frac{\Delta u_I}{2} < \ell n \frac{1}{\alpha} \leq \Delta u_I$
3	$\ell n \frac{1}{\alpha} > u_I$

The lethargy gain indicator is used in the correction of the elastic removal cross section for the actual flux spectrum in a specified reactor region (i.e., the correction of the elastic removal cross section in the generalized file which is output by ENDRUN). This correction can be described by referring to the diagram below which shows a sample flux distribution across coarse groups.



A lethargy indicator for coarse group I has the following connotation.

Lethargy gain indicator = 1

The elastic removal cross section is corrected between $u_{U,I}$ and $u_{U,I} - \Delta u_I/2$ based upon a flux interpolation between ϕ_I and ϕ_{I+1}.

Lethargy gain indicator = 2

The elastic removal cross section is corrected between $u_{U,I}$ and $u_{U,I} - (\Delta u)_I/2$ based upon a flux interpolation between ϕ_I and ϕ_{I+1}, and corrected between $u_{U,I} - (\Delta u)_I/2$ and $u_{U,I} - \ell n\frac{1}{\alpha}$ based upon a flux interpolation between ϕ_I and ϕ_{I-1}.

Lethargy gain indicator = 3

The elastic removal cross section is corrected between $u_{U,I}$ and $u_{U,I} - (\Delta u)_I/2$ based upon a flux interpolation between ϕ_I and ϕ_{I+1}, and corrected between $u_{U,I} - (\Delta u)_I/2$ and $u_{U,I-1}$ based upon a flux interpolation between ϕ_I and ϕ_{I-1}.

The analytical formulation for correcting the elastic removal term is different for each indicator and is described in TDOWN (reference 5).

3.4.5 Scattering from Hydrogen

For the special case of elastic scattering from hydrogen, the removal expression for coarse group I is given as,

$$\sigma_{er_I} = \frac{\sum_j \sigma_{e_j} \phi_j \; e^{-(u_{U,I} - u_{U,j})} \left(\frac{1 - e^{-\Delta u_j}}{\Delta u_j} \right)}{\sum_j \phi_j} \qquad 4.24$$

where the summation is over all fine groups j in coarse group I and the remaining terms are defined in Section 3.4.3.

The downscattering terms for coarse group I to coarse group M are the following,

$$\sigma_{er}(I \to M) = \sigma_{er,I} \; e^{-(u_{L,M} - u_{U,I})} [1 - e^{-(\Delta u)_m}] \qquad 4.25$$

If the downscattering matrix is truncated the last transfer term will be given by,

$$\sigma_{er}(I \to M^{max}) = \sigma_{er,I} - \sum_{L=I+1}^{M^{max}-1} \sigma_{er}(I \to L) \qquad 4.26$$

3.5 REACTION PARAMETERS

Reaction parameters which are generated from the ENDF/B data include: (1) the average cosine for elastic scattering, μ; (2) the average logarithmic energy decrement, ξ; (3) the number of neutrons emitted per fission, ν; and (4) the average fission spectrum fraction, χ.

3.5.1 Average Cosine of the Scattering Angle, μ, and Average Logarithmic Energy Loss, ξ

Pointwise data for μ and ξ are given in File 3 of the ENDF/B library and are processed like the data for the infinitely-dilute reaction cross sections. That is, the pointwise data are interpolated to the mid-lethargy energy for fine group j and are weighted by the fine group flux and summed as follows:

$$\langle \mu \rangle_I = \frac{\sum_j \mu_j \phi_j}{\sum_j \phi_j} \qquad 5.1$$

and

$$\langle \xi \rangle_I = \frac{\sum_j \xi_j \phi_j}{\sum_j \phi_j} \qquad 5.2$$

where the summation is over all fine groups j in coarse group I.

If elastic scattering cross section data is not available or has not been requested by the user the calculations for μ and ξ, which represent only a rough approximation, will be completed. However, since both μ and ξ are given meaning only in the process of elastic scattering, the average of these quantities will depend not only on the reaction variables but also on the relative elastic cross section at each energy. Thus, the fine groups are later reaveraged (if the data is available and after resolved and unresolved resonance contributions to σ_s have been calculated) and the

final coarse group average is given by:

$$\langle \mu \rangle_I = \frac{\sum_j \mu_j \sigma_{s_j} \phi_j}{\sum_j \sigma_{s_j} \phi_j} \qquad 5.3$$

and

$$\langle \xi \rangle_I = \frac{\sum_j \xi_j \sigma_{s_j} \phi_j}{\sum_j \sigma_{s_j} \phi_j} \qquad 5.4$$

If the pointwise data for ξ are not available, a special input option in ENDRUN can be used to carry out a theoretical calculation of ξ according to

$$\xi = 1 + \left(\frac{\alpha}{1-\alpha}\right) \ell n \alpha \qquad 5.5$$

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

and A = atomic weight

An average over the fine group values of $(1-\mu)\sigma_s$, normalized to the theoretical approximation $(1-2/3A)\sigma_s$, then provides a correction to account for the effects of anisotropy and yields the final average for coarse group I,

$$\langle \xi \rangle_I = \frac{\xi \langle (1-\mu)\sigma_s \rangle_I}{(1-2/3A)\langle \sigma_s \rangle_I} = \frac{\xi \sum_j (1-\mu_j)\sigma_{s_j}\phi_j \Big/ \sum_j \phi_j}{(1-2/3A) \sum_j \sigma_{s_j}\phi_j \Big/ \sum_j \phi_j} \qquad 5.6$$

3.5.2 Average Number of Neutrons Emitted Per Fission, ν

Data for the average number of neutrons per fission, ν, are given in File 1 of the ENDF/B library in either of two ways: (1) coefficients for a polynomial of degree N or (2) a tabulated, pointwise representation. In either case, the processing of the data is similar to the processing of the data for μ and ξ in the previous section. Values of ν are calculated - from the polynomial equation or by interpolation - at each mid-lethargy energy for fine group j. Since ν has meaning only in connection with a fission reaction, the group average value will depend upon the relative fission cross section at each energy. The final coarse group average of ν is fission weighted as follows:

$$\langle \nu \rangle_I = \frac{\sum_j \nu_j \sigma_{f_j} \phi_j}{\sum_j \sigma_{f_j} \phi_j} \qquad 5.7$$

3.5.3 Average Fission Spectrum Fraction, χ

The average fission spectrum fraction, χ, is calculated from the data in File 5 of the ENDF/B library. The data consists of tabulated probability functions and a range of nuclear temperatures with or without additional constants. The temperature, θ, may be given as an energy dependent parameter and for this case the temperature may be interpolated to an input energy specified by the user.

The χ values are calculated according to one of the following analytical expressions:

Fission Spectrum

$$\chi(E) = \sqrt{\frac{4E}{\pi\theta^3}}\ e^{-E/\theta}$$

Maxwellian Spectrum

$$\chi(E) = (E/\theta^2)\ e^{-E/\theta}$$

Watt Spectrum

$$\chi(E) = \sqrt{\frac{4}{\pi a^3 b}}\ e^{-ab/4}\ e^{-E/a}\ \sinh\sqrt{bE}$$

The ENDRUN calculation uses only a simple pointwise average. Thus, $\chi(E)$ and $P(E)$ are calculated and/or interpolated to each of the fine group mid-lethargy energy values and the integration is approximated by the following summation

$$\langle \chi \rangle_I = \sum_j \chi_j P_j E_j \Delta u_j \qquad 5.8$$

The $\langle \chi \rangle_I$ values are then normalized to 1.0.

3.6 OVERLAP CORRECTIONS

Several different types of cross section overlap are possible, some inherent to the physics of averaging calculations, others due to the generalized ENDF/B format which allows different types of data to be given for the same reaction at the same energy. In particular, the following types of overlap may be processed by the ENDRUN code:

(1) Statistical resonance overlap within unresolved resonance calculations -- discussed in Section 3.3 and processed as an option according to the Nicholson "A" method (Reference 1).

(2) Overlap of unresolved resonance sequences.

(3) Overlap of unresolved and resolved resonance data in the same coarse group.

(4) Overlap of unresolved and/or resolved resonance data with smooth, pointwise contributions.

All of these overlap situations have in common the combination of two or more sets of cross section data which have been separately averaged over a coarse group. In the infinitely dilute case, in which only the coarse flux is used for weighting, these separately averaged quantities can be combined by a simple summation, i.e.

$$\langle \sigma_x^\infty \rangle_I = \langle \sigma_x^\infty \rangle_{I_{smooth}} + \langle \sigma_x^\infty \rangle_{I_{unresolved}} + \langle \sigma_x^\infty \rangle_{I_{resolved}} \qquad 6.1$$

Similarly, unresolved resonance sequences, k, can be summed to give:

$$\langle \sigma_x^{\infty} \rangle_I = \sum_{c=1}^{N} \langle \sigma_x^{\infty} \rangle_I^c \qquad 6.2$$

When self-shielding is required, however, the fine flux $(1/\sigma_t+\sigma_o)$ for each calculation is different (e.g. the total cross section in unresolved resonance averaging is only the unresolved contribution to total). Since σ_t is thus too small, the self-shielded values are actually for different -- and smaller -- effective σ_o's. One way to correct this situation is to first determine the correct σ_t and then adjust each self-shielded value by interpolating to the correct effective σ_o. Fortunately, temperature remains the same in all cases, so only a one-step interpolation is necessary. This interpolation is based upon a Taylor expansion about the original σ_o value.

3.6.1 F-Factor Interpolation

The interpolation scheme employed by ENDRUN for correcting the self-shielded cross section is based upon a Taylor series expansion of the f-factors in terms of $\ell n\ \sigma_o$. A typical plot of f_i vs x (actually f_c for U-238) is given in Figure 3.1 where:

$$f_i(\sigma_o) = \frac{\sigma_i(\sigma_o)}{\sigma_i(\infty)} \qquad \text{(for reaction type i)}$$

and

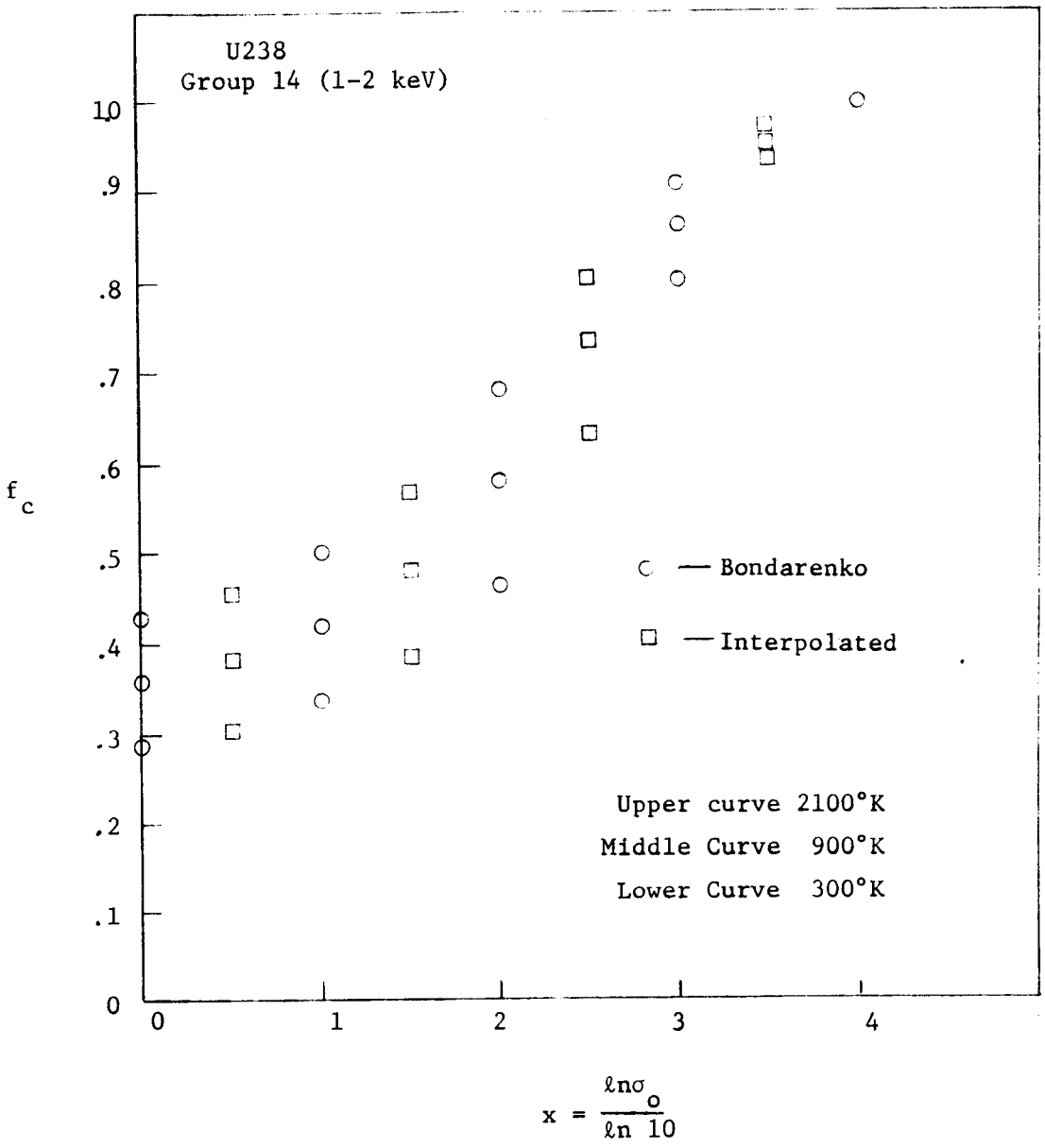
$$x = \frac{\ell n\ \sigma_o}{\ell n\ 10}$$

Although the graph stops at x = 0 or σ_o = 1.0, σ_o values closer to 0 are possible; the only restriction is that the logarithmic intervals between two different values of σ_o must be constant (i.e. consecutive values of σ_o must be multiples of the same constant).

If we assume that f has been calculated for values x_1, x_2, x_3, x_4 and

FIGURE 3.1

CURVES OF SELF-SHIELDING FACTORS AS FUNCTIONS OF σ_o



that f = 1.0 at x_5, then the interpolated value of f at x, a distance δ from x_3, may be found by expanding the Taylor series around the closest values (e.g. around x_3 and x_4) and weighting inversely with the distance from each point. The Taylor series expansion of f at x about x_n is:

$$f(x) \cong f(x_n+\delta) = f(x_n) + \left(\frac{df}{dx}\right)_n \delta + \left(\frac{d^2f}{dx^2}\right)_n \frac{\delta^2}{2} + \ldots\ldots \qquad 6.3$$

Evaluation of these derivatives will depend on the location of x with regard to x_{min} and x_{max}, the minimum and maximum values of x in a given ENDRUN calculation. Interpolation results in one of the following 5 cases:

1) $\underline{x \leq x_{min}}$

$$f(x) = f(x_{min})$$

2) $\underline{x \geq x_{max} + \Delta}$

$$f(x) = 1.0$$

3) $\underline{x_{min} < x \leq x_{min} + \Delta}$

$$f(x) = f(x_{min}+\Delta)\left[1 - \left(\frac{\delta_1}{\Delta}\right)^2\right] + f(x_{min})\left[\frac{1}{2}\left(\frac{\delta_1}{\Delta}\right)^2 - \frac{1}{2}\frac{\delta_1}{\Delta}\right] + f(x_{min}+2\Delta)\left[\frac{1}{2}\left(\frac{\delta_1}{\Delta}\right)^2 + \frac{1}{2}\frac{\delta_1}{\Delta}\right] \qquad 6.4$$

where: $\delta_1 = x_{min}+\Delta-x$

and if $f(x) < f(x_{min})$ $f(x)$ is set = $f(x_{min})$.

4) $\underline{x_{max} \leq x \leq x_{max} + \Delta}$

$$f(x) = f(x_{max})\left[1 - \left(\frac{\delta_2}{\Delta}\right)^2\right] + f(x_{max}-\Delta)\left[\frac{1}{2}\left(\frac{\delta_2}{\Delta}\right)^2 - \frac{1}{2}\left(\frac{\delta_2}{\Delta}\right)\right] + 1\left[\frac{1}{2}\left(\frac{\delta_2}{\Delta}\right)^2 + \frac{1}{2}\frac{\delta_2}{\Delta}\right] \qquad 6.5$$

where: $\delta_2 = x - x_{max}$

and if $f(x_{max}) < 1$ and $f(x) > 1$, $f(x)$ is set = 1.0

if $f(x_{max}) > 1$ and $f(x) > f(x_{max})$, $f(x)$ is set = $f(x_{max})$

(5) $x_{min} + \Delta < x < x_{max}$

locate n such that $x_n \leq x < x_{n+1}$

$$f(x) = \frac{x_{n+1}-x}{\Delta} f_{x,n} + \frac{x-x_n}{\Delta} f_{x,n+1}$$

where: $$f_{x,n} = f(x_n)\left[1 - \left(\frac{\delta_3}{\Delta}\right)^2\right] + f(x_{n-1})\left[\frac{1}{2}\left(\frac{\delta_3}{\Delta}\right)^2 - \frac{1}{2}\frac{\delta_3}{\Delta}\right]$$

$$+ f(x_{n+1})\left[\frac{1}{2}\left(\frac{\delta_3}{\Delta}\right)^2 + \frac{1}{2}\frac{\delta_3}{\Delta}\right] \qquad 6.6$$

for: $\delta_3 = x-x_n$

and $$f_{x,n+1} = f(x_{n+1})\left[1 - \left(\frac{\delta_4}{\Delta}\right)^2\right] + f(x_n)\left[\frac{1}{2}\left(\frac{\delta_4}{\Delta}\right)^2 - \frac{1}{2}\frac{\delta_4}{\Delta}\right]$$

$$+ f(x_{n+2})\left[\frac{1}{2}\left(\frac{\delta_4}{\Delta}\right)^2 + \frac{1}{2}\frac{\delta_4}{\Delta}\right] \qquad 6.7$$

for: $\delta_4 = x-x_{n+1}$

Although the detailed equations for overlap corrections are shown below only for the case of unresolved resonance sequences; the method is essentially the same for all overlap situations.

3.6.2 Combining Unresolved Resonance Sequences

The contribution of each unresolved resonance sequence of a given isotope to the energy averaged cross section for reaction type χ, at each energy point and for each σ_o and temperature is computed by neglecting a term in the total cross section - namely the contribution of the other resonance sequences,

$$\sum_{\substack{c'=1 \\ c'\neq c}}^{N} \left\langle \sigma_{T,c'} \right\rangle \qquad 6.8$$

which is taken to be constant in energy across a resonance spacing. That is, the resonance integrals are originally computed with a flux approximation of the form

$$\phi(E) \simeq \frac{1}{\sigma_{T,c}(E)+\sigma_p(E)+\sigma_o} \qquad 6.9$$

The missing portion of the total cross section may be treated as an addition to σ_o, and the resonance contribution adjusted to the correct value for the desired σ_o.

A Taylor expansion about $\ell n\ \sigma_o$ is then used to determine the energy average cross section which would have been computed with a flux of the more complete form,

$$\phi(E) = \frac{1}{\sigma_{T,C}(E)+\sigma_p(E) + \sum_{\substack{c'=1 \\ c'\neq c}}^{N} \left\langle \sigma_{T,c'} \right\rangle + \sigma_o} \qquad 6.10$$

The corrected values of the cross section are then summed over all resonance sequences for each energy point, σ_o, temperature and reaction type.

3.6.3 Resolved-Unresolved Resonance Range Overlap

If the contributions from resolved and unresolved resonances overlap in energy across a full coarse group, the standard overlap correction as described in Section 3.6.2 is applied. This provides a first order correction for the effects of each contribution on the total cross section seen by the other. However, in the coarse groups for which one or both the unresolved and resolved ranges end, special attention must be given to the correction. Since one or both of the contributions do not apply over the entire coarse group, it would be incorrect to use group-average total cross sections to correct the self-shielding. The most important situation of this type involves the effect of the unresolved contribution on the resolved self-shielding when the two energy ranges butt against one another. In this case, nearly the complete cross section contribution is transferred from the resolved to unresolved resonances, and, since large energy variations are likely to exist in the resolved cross sections, sizeable errors could exist with the standard correction. If the two ranges actually overlap, it is most likely that one or the other will dominate and the overlap correction will be less important.

In order to deal specifically with the case where the two ranges butt against each other, fine group values of σ_t are retained for the lowest-energy group of the unresolved range and are used directly in self-shielding of the resolved resonances. Later, when all contributions are summed and the standard corrections made, the correction to the resolved portion of this boundary group is bypassed to avoid redundancy. The self-shielded unresolved portion is still corrected since the resolved contribution to the total cross section was not available at the time of the original calculation.

For the cases where both resolved and unresolved ranges do not end in the same coarse group, but still overlap, this special method is again applied to the lowest-energy unresolved group. The standard correction is applied to the highest-energy resolved group.

SECTION IV

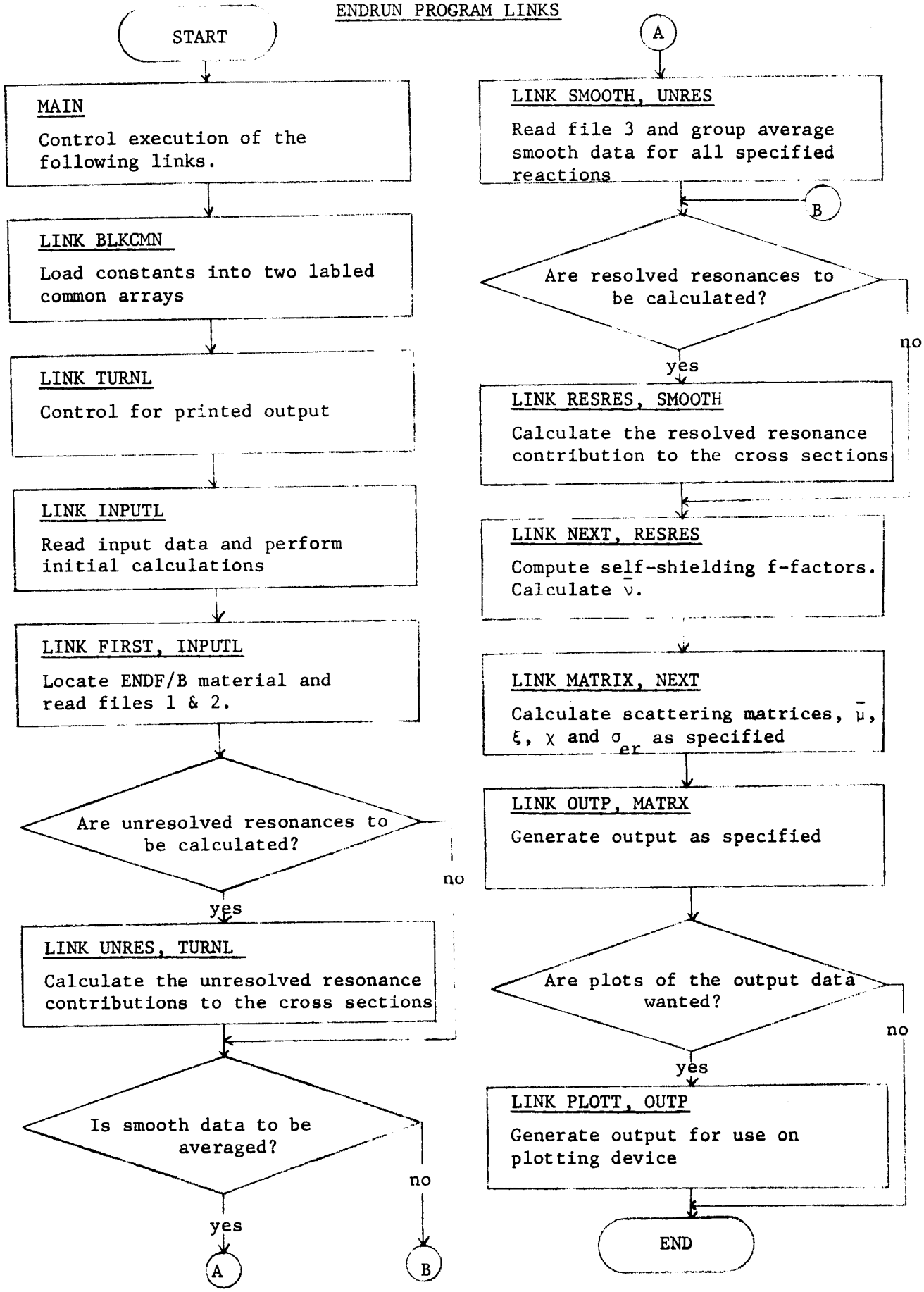
PROGRAM DESCRIPTION

The ENDRUN program consists of a main program and eleven links. The linking system allows the overlay of coding so that separate data types are processed with only the necessary programming in the computer. The computer memory requirements are minimized in this manner.

The broad program logic is illustrated in Figure 4.1. In the illustration some links have two names; the second name specifies the link overlaid by the first. Following Figure 4.1 is a description of the MAIN program and each link. For a more detailed description of the links and the subroutines in ENDRUN the user is referred to the ENDRUN Programmers Manual[12].

FIGURE IV-1

ENDRUN PROGRAM LINKS



MAIN — The MAIN routine directs the sequential execution of the code and contains the blank and labeled common used for transferring data from link to link. The subroutines in MAIN are always in memory so they are available for use in other links. These subroutines are used primarily for locating, reading and interpolating data in the ENDF/B libraries.

BLKCMN — This link contains a block data routine which loads several constants into labeled common for use in other subroutines.

TURNL — The routine in TURNL controls the format of the input edit.

INPUTL — The input data is read, checked and loaded into memory in this link. Initial calculations are carried out to prepare the input data into the arrays which are necessary for the execution of other links.

FIRST — The ENDF/B material is located and written onto a disc in FIRST. Resonance data is written on another disc for use in the resonance calculations. The fine group energies and fluxes are also calculated in this link.

UNRES — The unresolved resonance contribution to the total, scattering, capture and fission cross sections are computed in this link. The unresolved infinitely-dilute and self-shielded contributions are calculated at the energy points specified by the user; then the pointwise cross sections are flux averaged for all coarse groups.

SMOOTH — The pointwise cross sections are averaged over fine groups after interpolation of the data to the mid-lethargy energy values of the fine groups. Self-shielding of the smooth cross sections is also done in SMOOTH.

RESRES — The resolved resonance contribution to each fine group is calculated and added to the appropriate smooth data in this link. The output of this link includes the fine and coarse group cross sections in the resolved range for all temperatures and σ_o's.

NEXT — The self-shielding factors are calculated in NEXT based on contributions from unresolved, resolved and smooth data to the cross sections. The average number of neutrons per fission, ν, is also calculated in this link.

MATRIX — This link contains routines for generating the inelastic, n-2n and elastic scattering matrices. Group average values for μ (average cosine of the elastic scattering angle), χ (fraction of fission neutrons within a coarse group), and σ_{er} (elastic removal cross section) are computed in this link.

OUTP — The OUTP link generates the four types of output available in ENDRUN. The output subroutines are briefly described as follows:

OUTPUT - subroutine for printing all group averaged cross sections, self-shielding factors and scattering matrices.

FCCOUT - subroutine for punching cross sections to be used in fixed format codes.

TROUT - subroutine for punching infinitely-dilute cross sections on cards.

STDOUT - subroutine generates a one-material GMUG file on tape for use in the TDOWN code.

PLOTT — Data is arranged into the format required by the series of subroutines called DRAW, the GE general purpose plotting routine.

SECTION V

INPUT DESCRIPTION

5.1 CONTROL CARDS

The following control cards are required on the GE-635 unless otherwise noted.

Card Column:	1	8	16
CARD PURPOSE			
Job Identification	$	IDENT	CCCC,III-locat,ENDRUN
Program loader	$	PROGRAM	RLHS
ENDRUN program	$	TAPE	H*,H1DD,,MMMM,,ENDRUN H*
Program limits	$	LIMITS	tt,53K,10000,10000
Peripheral storage	$	FILE	01,,25L (Tape Optional)
Peripheral storage	$	FILE	02,,5L
Peripheral storage	$	FILE	03,,5L
Peripheral storage	$	FILE	04,,10L
Output file (print)	$	SYSOUT	06
Input file (ENDF/B tape)	$	TAPE	07,N1DD,,MMMM,,NPOST ENDF/B (optional)
Peripheral storage	$	FILE	08,,5L
Peripheral storage	$	FILE	09,,5L
Peripheral storage	$	FILE	10,,2L
Input file (QUICKW tape)	$	TAPE	11,Q1DD,,MMMM,,QUICKW TABLE (optional)
Output file (GMUG tape)	$	TAPE	12,G1DD,,,,GMUG MAT. (optional)
Peripheral storage	$	FILE	13,,1L
Peripheral storage	$	FILE	14,,25L
Peripheral storage	$	FILE	15,,1L
Output file (PLOT tape)	$	TAPE	39,P1D,,,,PLOT TAPE (optional)
Output file (cards)	$	SYSOUT	43 (optional)
Transliteration card	$	INCODE	IBMF
Conclusion of job	$	ENDJOB	

CCCC = user's charge number
III-locat - user's initials and location
MMMM - tape reel number
tt - maximum problem run time in hundredths of an hour

All TAPE, FILE and SYSOUT control cards use file code numbers so reference can be made to the files. The alphanumeric file code number is designated in card columns 16 and 17.

Several of the above peripheral file control cards are optional. These cards and their uses are listed in Table 5.1.

TABLE 5.1

OPTIONAL CONTROL CARDS

File Code	Use
01	ENDF/B data tape, either BCD (for one material only) or binary. May be a disc if using an NPOST tape on 07 or may be omitted if running from cards.
07	NPOST compressed binary tape containing complete ENDF/B data file. Desired material is read on to File Code 01 before actual use.
11	QUICKW table, permanently saved on tape. May be generated by ANL routines WL and W (Reference 9).
12	GMUG tape generated for a single material at the end of an ENDRUN case and saved to be added to the GMUG file
39	Plotting tape - save temporarily to obtain X-Y plots of cross sections or f-factors.
43	Punched card output

If any optional file is not needed, that control card may be omitted.

5.2 DATA CARDS

The data cards must be preceded by a CASE card and followed by a LAST card as shown below.

Card column:	1	6	9	28
CASE Card	)ENDR	iii	*nnnnn	ddddddd
Data Cards				
LAST card	)LAST		*	

iii = user's initials

nnnnn = case name

ddddddd = date

(Columns 6 to 34 may be left blank)

The ENDRUN input data are given in the free format except for several optional data sets which are input in the fixed format. Free form data cards have the following content:

COLUMN	CONTENT
1-12	Card type
13-15	ii
21-80	free form data

The card type is represented by an alphanumeric name (left justified in columns 1 to 12). Associated with the card type is a data set for which the input values are listed (in order) in columns 21 to 80. More than one card may be included for a specific data set and the beginning location of the data will be specified by ii in columns 13-15. If ii is left blank, it is assumed to be one greater than the last, previously filled location in that data set. Any card which immediately follows a card of the same type may use an asterisk in column 2 rather than the entire card type name in columns 1 to 12.

The data in columns 21 to 80 must be separated by one or more blanks or a comma, and comments may be included if they are enclosed in parenthesis and are separated from the numerical data by one or more blanks. The cards are processed one at a time so a number or a comment cannot continue from one card to the next. A number may be loaded into n

consecutive locations of the data set if it is followed by one or more blanks, or a comma, and then an Rn or a *n. Sn or /n preceded by a blank will indicate that n consecutive locations in the data set be skipped over without altering their contents. Consecutive commas or a leading comma cause integer zeros to be loaded.

Values for several data sets (e.g. TEMPERATURES) are input as a list of arbitrary length. These values must be loaded into consecutive locations beginning with the first available location and the end of the list is indicated by the first zero.

The following card types are currently available for ENDRUN. The names of the data set entries shown are generally those used in the FORTRAN instructions. They are preceded by an (i) if they must be input as integers and by an (a) if they are alphanumeric. nH must precede any n characters of alphanumeric input (including blanks). All other input numbers require a decimal point and may be followed (without separating blanks) by an exponent of the form EΔ±n. The EΔ need not be included; or if the E is given, the Δ and/or the sign need not be given.†

If a data set entry is omitted from input it will be assigned the value of zero.

Card type name	ii	Data Set Entry Name	Entry Description
TITLE	1-20	(a) IDENT	120-character case identification. Six characters per entry. Note that any number of TITLE cards may be included to identify the case, but only the first 120 characters will be printed in the output. TITLE cards may be omitted if none are wanted.
GENERAL	1	(i)MATT	Material number on ENDF/B file.
	2	(i)LRECD	ENDF/B file type indicator = 0; cards = 1; binary tape = 2; NPOST tape = 3; BCD tape

† n = an integer
Δ = a one-character blank

Card type Name	ii	Data Set Entry Name	Entry Description
			If ENDF/B data is read from an NPOST (GE compressed binary) tape, ENDRUN actually creates an intermediate BCD file (for one material) which may be saved on file code 01. This tape could later be used by setting LRECD=3. Recommended procedure is to use DAMMET to create a large ENDF/B binary file and run ENDRUN from that if a compressed binary system such as NPOST is not available.
	3	(i)ITOT	Total number of coarse groups. $1 \leq ITOT \leq 100$.
	4	(i)IMIN	Number of the lowest coarse group (highest energy) to be calculated.
	5	(i)IMAX	Number of the highest coarse group (lowest energy) to be calculated.
	6	SLETH	Starting lethargy. SLETH is 0.0 for a starting energy of 10 MeV, but can be negative to yield a higher beginning energy.
	7	FSCL	Energy at which flux-weighting spectrum changes from 1/E to Maxwellian distribution (in MeV).
	8	TMW	Temperature in MeV of Maxwellian spectrum.
	9	FRAC	Fraction of group lethargy width used in calculating the elastic removal cross sections.
	10	(i)MNOG	Material number on GMUG file.
OPTIONS			Indicators which select various optional calculations are included in this data set.
	1	(i)SMOOTH	= 1; do <u>not</u> calculate smooth cross section contribution. = 0; do
	2	(i)NU	= 1; do ν calculations = 0; do not

Card type Name	ii	Data Set Entry Name	Entry Description
			If NU=1, the material must be fissionable and ICT=4 must be specified on a REACTIONS card so that fine group fission cross sections are available for weighting of $\bar{\nu}$.
	3	(i)NSTOT	=1; adjust σ_{es} for balance and put ENDF/B total on file (not available). = 0; adjust total cross sections on file to equal sum of partials.
	4	(i)NSPOPT	=1; calculate self-shielding factors using ICT=5 as the total cross section (not available). =0; calculate self-shielding factors using ICT=1 as the total cross section.
	5	(i)IRUN	=1; case will be executed even if non-fatal input errors are found. =0; execution will be terminated if any input errors are found.
OUTPUT			Special output requirements are specified in this data set. It may be omitted if only the automatic printout is wanted.
	1	(i)LOUT(1)	=1; GMUG file created on File Code 12 =0; No GMUG file (and no tape needed on FC12)
	2	(i)LOUT(2)	=1; punched card output in DTF (6E12.6) format. =2; output on tape (not available).
	3	(i)LOUT(3)	=1; punched cards in TROUT format (infinitely dilute averages and combined matrix only).
	4	(i)LOUT(4)	=1; Plotted output of coarse group averages or f-factors.
	5	(i)LOUT(5)	=1; fine group energies and fluxes used in averaging are printed out.
	6	(i)LOUT(6)	=1; Unresolved resonance contributions are printed as a function of ℓ,j at each energy point and for all coarse groups. =2; Fine group interpolated unresolved contributions are also printed.

Card type Name	ii	Data Set Entry Name	Entry Description
	7	(i)LOUT(7)	=1; ENDF/B file 3 data is printed out as it is read.
	8	(i)LOUT(8)	=1; coarse group averages for single reaction types (MT) are printed as they are calculated in addition to the automatic output of reaction type ICT averages (smooth region only). =2; fine group cross sections are printed as calculated.
	9	(i)LOUT(9)	=1; self-shielded coarse group averages are printed as they are calculated (smooth region only).
	10	(i)LOUT(10)	Intermediate smooth plus resolved resonance cross section contribution edit indicator =0; none =1; coarse groups (infinitely dilute and self-shielded) =2; coarse groups and fine group infinitely dilute =3; coarse and fine groups (infinitely dilute and self-shielded).
	11	(i)LOUT(11)	=1; intermediate printout of fine group values of ν and $\nu\sigma_f$.
	12	(i)LOUT(12)	Not specified at present.
	13	(i)LOUT(13)	=1; matrix changes due to renormalization are printed out.
	14	(i)LOUT(14)	Not specified at present.
	15	(i)LOUT(15)	Not specified at present.
	16	(a)MFIL	Alphanumeric material name - printed on plots and punched on TROUT and FCC cards.

Automatic printed output from ENDRUN includes a listing of input cards, a table of coarse group energies, lethargy widths and f-factor control numbers and the final coarse group averages for all output reaction types, f-factors, and matrices. The output control numbers in this data set are in addition to the automatic printout. The first three control numbers provide punched or tape output for direct use with other codes: a GMUG

file for the TDOWN code; punched cards with f-factors for the Battelle FCC-IV code; and punched cards without f-factors for a standard MUG file.

Card type Name	ii	Data Set Entry Name	Entry Description
REACTIONS	The ENDF/B reaction types (MT) which are to be included in any of the ENDRUN output reaction types (ICT) are specified in this data set. For this card type, ii is the ICT value and jj (Column 17-18) is used as a counter for reaction types requiring more than one card.		
	ICT	(i)$MCRS_{ICT,\ell}$	List the ENDF/B reaction types to be included in ENDRUN output reaction type. See ICT list below.

ICT	Reaction Meaning
1	Total cross section = sum of partials
2	Elastic scattering
3	Capture, may include (n,γ), (n,p), (n,α)
4	Fission
5	Total cross section, as given by ENDF/B
6	Inelastic
7	Xi = average lethargy loss by elastic scattering (ξ)
8	Mu = average cosine of elastic scattering angle (μ)
9	(n,2n)
10	(n,3n)
11	Nu = average number of neutrons released per fission (ν)
12	Elastic removal σ_{er}
13	Chi = fraction of fission neutrons arriving in this energy group (χ)

ICT	Reaction Meaning
14	LGI = lethargy gain indicator = 1.0, $\ell n\frac{1}{\alpha} \leq \Delta u/2$ = 2.0, $\ell n\frac{1}{\alpha} > \Delta u/2$ = 3.0, $\ell n\frac{1}{\alpha} > \Delta u$
15	Blank at present.

Output reactions 11 to 15 are handled differently from those numbered 1 to 10 and should not be specified in this data set. Any reaction types 1 to 10 which are not specified in this data set will not be calculated.

ENDRUN allows combinations of several input reaction types (MT values) in a single output type, e.g. (n,γ) (MT=102) and (n,α) (MT=107) in capture (ICT=3). The only restrictions are: 1) Any MT value can appear in only one output reaction other than the total; 2) No more than 15 MT values can be combined in one output reaction; 3) If two or more MT values are combined in one output reaction the corresponding combined MT value (i.e. absorption) should not be used elsewhere; 4) If two MT values are combined and both have secondary energy distributions, only the first distribution will be used in matrix calculations and it will be weighted by the combined cross sections, not that of its separate MT value. Thus, even if a combined inelastic and (n,2n) matrix is desired, inelastic and (n,2n) reactions should be treated separately with two REACTIONS cards; 5) If the inelastic cross sections are given by levels in file 3, only the first and last MT values for the levels should be input in the ICT=6 REACTIONS card.

Card type Name	ii	Data Set Entry Name	Entry Description
DELTA U/CG			The lethargy width of each coarse group is specified in this data set.
	3ℓ-2	$DELU_\ell$	Δu of each coarse group in sequence ℓ.
	(i)	$IFIRST_\ell$	Beginning coarse group in sequence ℓ.
	(i)	$ILAST_\ell$	Last coarse group in sequence ℓ.
			Repeat ($DELU_\ell$, $IFIRST_\ell$, $ILAST_\ell$) for ℓ=1 to the number of sequences on the card.

The coarse group structure to be used is input as sequences of group lethargy widths. The lower energies of each group are then computed based on the starting lethargy given on the GENERAL card. The lethargy width, ΔU, of each coarse group in sequence ℓ, is assumed to be constant between groups IFIRST and ILAST. Any number of DELTA U/CG cards may be given, and each card may contain as many sequences as will fit, but the three numbers describing any sequence must all be on the same card.

FINE GPS/CG			The number of fine groups in each coarse group is specified in this data set.
	3ℓ-2	(i)NFG_ℓ	Number of fine groups per coarse group in sequence ℓ $1 \leq NFG \leq 30$
		(i)$IFIRST_\ell$	Beginning coarse group in sequence ℓ
		(i)$ILAST_\ell$	Last coarse group in sequence ℓ
			Repeat (NFG, IFIRST, ILAST) as necessary.

Any number of FINE GPS/CG cards may be given, and each card may contain as many sequences as will fit, but the three numbers describing any sequence must all be on the same card.

SIGMA-NOUGHT			Parameters representing other-material cross sections (σ_o's) used for computing a generalized self-shielding table of f-factors are specified in this data set. It may be omitted if f-factors are not wanted.
	ℓ	SGO_ℓ	List σ_o values (in ascending order). $2 \leq \ell \leq 5$.

Card type Name	ii	Data Set Entry Name	Entry Description
			Because of the interpolation routine used in adjusting the self-shielding for overlapping sequences and data types, the ratio (logarithmic or linear) of consecutive σ_o values must be constant, e.g. 1.0 - 10.0 - 100.0 or 20 - 40 - 80, and at least two σ_o values must be input if this option is used.
F-F SMOOTH			Coarse groups for smooth data f-factors are specified in this data set. They may be omitted if f-factors are not wanted.
	$2\ell-1$	(i)IFIRST$_\ell$	Smooth data f-factors will be calculated for groups IFIRST to ILAST. F-factor calculations are always made for total, capture, scattering, and fission (if given) cross sections so no reaction specification need be made.
		(i) ILAST$_\ell$	
			Repeat (IFIRST, ILAST) as necessary.
TEMPERATURES			Temperatures used in the resonance calculations are specified in this data set. They may be omitted if f-factors are not wanted.
	ℓ	TT$_\ell$	List temperatures in degrees-Kelvin. (In ascending order). $1 \leq \ell \leq 3$
			A temperature of 300°K is automatically used for resonance calculations if no temperature is input.
UNRESOLVED R			Input for the unresolved resonance calculations is specified in this data set. It may be omitted if no unresolved resonance calculations are wanted.
	1	(i)NDELIF	=0; Do not punch unresolved results on cards. =1; Punch pointwise unresolved contributions to infinitely dilute and self-shielded cross sections.
	2	(i)LFLUXC	
	3	(i)LAPC	=1; Unresolved resonance self-overlap corrections for self-shielding (reference 4)

Card type Name	ii	Data Set Entry Name	Entry Description
	4	ELAPC	Do not perform overlap correction below this energy (in eV).
	5	(i)NUNDU	Number of energy points in unresolved range. $3 \leq$ NUNDU ≤ 30 It is suggested that the user select all or some of the energy points where the unresolved parameters are given on the ENDF/B file.
	6	URR_1	Lowest energy of the unresolved region. (in eV). (automatically set to ESS, if not input)
	7	URR_2	Energy above which f-factors are not needed. (in eV). (automatically set to ESS, if not input)
	8	URR_3	Highest energy of unresolved region (in eV) (automatically set to ESS_{NUNDU} if not input)
	9	ESS_1	Lowest energy at which an unresolved calculation is desired (in eV).
	10	ESS_2	Next energy point
	NUNDU+8	ESS_{NUNDU}	Last energy point.

Unresolved resonance calculations are performed at NUNDU energy points which depend only on the ENDF/B input range and not on the coarse group structure of a particular ENDRUN case. The NDELIF = 1 option may, therefore, be used to punch cards with the unresolved contributions at these energies and future cases can be run directly from these cards at considerable savings of computer time.

LFLUXC specifies the type of unresolved calculation to be performed. The averaging techniques are briefly described by the general forms below.

Card type Name	ii	Data Set Entry Name	Entry Description
		LFLUXC	$\langle \sigma_x \rangle$
	0		$\left\langle \dfrac{\Gamma_{k,i} \int \frac{\sigma_x}{\sigma_x + \sigma_o} dx}{\Gamma_i \int \frac{dx}{\sigma_x + \sigma_o}} \right\rangle$
	1		$\dfrac{\langle \Gamma_{k,i} \int \frac{\sigma_x}{\sigma_x + \sigma_o} dx \rangle}{\langle \Gamma_i \int \frac{dx}{\sigma_x + \sigma_o} \rangle}$
	2		$\dfrac{(\sigma_p + \sigma_o)}{D} \left\langle \Gamma_{k,i} \int \frac{\sigma_x}{\sigma_x + \sigma_o} dx \right\rangle$

LFLUXC = 2 is recommended for general use, together with the self-overlap correction. In some cases LFLUXC = 1 gives more accurate results.

Self-shielding in the unresolved resonance region is further complicated by scattering interference and resonance overlap. The former is not considered in this version. Overlap of resonances of the same sequence may be considered with the LAPC = 1 option while first order corrections to the overlapping of resonances of different sequences (different ℓ,j states) is accounted for by an adjustment of σ_o.

Card type Name	ii	Data Set Entry Name	Entry Description
RESOLVED R			Control numbers for resolved resonance calculations are specified in this data set. It may be omitted if no resolved resonance calculations are wanted.
	3ℓ-2	(i)ISCON1$_\ell$	Resolved resonance contribution indicator in sequence ℓ 1 = No resolved contribution (this entire data set is initialized to 1 before cards are read). 2 = Resolved contribution, but no self-shielding necessary. 3 = Resolved contribution with self-shielding.
		(i)IFIRST$_\ell$	Beginning coarse group in sequence ℓ
		(i)ILAST$_\ell$	Last coarse group in sequence ℓ
			Repeat (ISCON1, IFIRST, ILAST) as necessary.
			Any number of RESOLVED R cards may be given and each card may contain as many sequences as will fit, but the three numbers describing any sequence must all be on the same card. The user should check the resolved resonance energy ranges in File 2 of ENDF/B data and specify the coarse groups in which resolved resonance data should be used to calculate the resolved contribution.
MATRIX			Data for matrix calculations are specified in this data set. If a particular matrix calculation is called for the corresponding smooth cross section must also be included.
	1	(i)INELAS	=1; generate inelastic matrix. If INELAS ≠ 0, ICT=6 must be specified on a REACTIONS card.
	2	(i)LN2N	=1; generate (n,2n) and/or (n,3n) matrix. If LN2N≠0, either ICT=9 or ICT=10 must be specified on REACTIONS cards.
	3	(i)LELASM	=1; generate elastic matrix and calculate σ_{er}.

Card type Name	ii	Data Set Entry Name	Entry Description
			If LELASM≠0, ICT=2 and ICT=7 or 8 must be specified on REACTIONS cards so that fine group values of σ_s and ξ are available.
	4	(i)LSEPM	=0; combine all matrices into inelastic matrix. =1; three separate matrices (inelastic, (n,2n), (n,3n) and elastic) If FCC or TROUT cards are desired, all matrices should be combined. (n,2n) and (n,3n) are combined even when LSEPM=1.
	5	(i)LDXI	=0; calculate $\bar{\xi}$ directly from ENDF/B File 3 MT=252 =1; calculate $\bar{\xi}$ and $\bar{\mu}$ allowing for anisotropy
	6	(i)ILINM	Highest numbered coarse group having an inelastic matrix (lowest energy group having inelastic scattering). Maximum number = 70.
	7	(i)NDSC	Maximum number of downscattering groups (for all matrices) (Maximum = 49)
	8	(i)ILNNM	Highest numbered coarse group having an (n,2n) matrix (lowest energy group having (n,2n) cross section). Maximum = 70.
	9	(i)LCHI	=1; calculate secondary fission neutron spectrum (group average χ values)
	10	(i)LECHI	=0; Use θ (nuclear temperature) energy given in ENDF/B File 5 = Nuclear temperature in KeV for use if several θ values are given.
	11	(i)LGP	Highest numbered coarse group to which downscattering can occur (only for TROUT card output). Maximum = 44.

Run costs may be reduced if the user checks ENDF/B File 5 for the threshold energies of inelastic and (n,2n) reactions. The corresponding coarse groups can be input as ILINM and ILNNM, respectively (upper limit = 70). The maximum number of downscattering groups (maximum = 49) will apply to all matrices. In the matrix normalization, any cross sections for scattering beyond the last downscattering

Card type Name	ii	Data Set Entry Name	Entry Description

group are added to the last scattering group. The matrix sum is normalized to the coarse group inelastic value, the difference being spread over the entire matrix. These normalization changes will be printed out if LOUT(13)=1 on the OUTPUT card.

The secondary fission neutron spectrum (χ) may be calculated, but the user must check that MT = 18 (fission) is given in ENDF/B File 5.

PLOT SIZES Miscellaneous control indices for plots are input in this data set. It may be omitted if LOUT(4) = 0 (on the OUTPUT card). It must be included if an INF-DIL PLOT or a F-FACTOR PLOT card is given in the deck.

1	(i)NSHEET	Number of separate plotting sheets. $1 \leq$ NSHEET ≤ 10.
		Plots must be specified for each of the NSHEET sheets on an INF-DIL PLOT and/or a F-FACTOR PLOT card.
	(i)ISIZE	Control size of grids = NIN(2)
		= +N X axis for N inches Y axis = 11 in.
		= -N Y axis of N inches X axis = 11 in.
		($8 \leq$ N ≤ 22)
		= 0 X axis = 11 in. Y axis = 8 in.
		= 1 X axis = 8 1/2 in. Y axis = 11 in.
	(i)IXGRID	= 0 draw internal grid lines
	(i)IYGRID	= 1 no internal gridding

Card type Name	ii	Data Set Entry Name	Entry Description
		(i)IKEY	Location of key array =0 no keys =1 upper left corner =2 upper right corner =3 lower left corner =4 lower right corner =5 above grid outside plot
INF-DIL PLOT	N	(i)ISTXI$_{\ell,N}$	List ICT values of infinite dilute curves wanted on the Nth plot sheet. ℓ = starting location of plot on sheet N, i.e. = 1 for first plot. Maximum ℓ = 5.
F-FACTR PLOT	N	(i)ISTX1$_{\ell,N}$	List ICT value
		(i)ISTX2$_{\ell,N}$	σ_o sequence number, and
		(i)ISTX3$_{\ell,N}$	Temperature sequence number for self-shielded curves wanted on the Nth plot sheet. Maximum ℓ = 6.

The plotting routine, PLOTXS, will probably require adaptation by every installation and thereby necessitate different input. The above, using the GE DRAW routine, is included for completeness.

INTRNL — Execution control constants which are normally defined within the code may be redefined through this data set.

1	EPS	The magnitude of resolved resonance contribution to the total cross section which a resonance must contribute to a group for its effect to be included in the resolved resonance calculations for that group. Set at .0001.
2	ACCINT	Relative accuracy wanted in resolved resonance integral calculations. Set at .005.
3	CLOSE	Relative accuracy required between NCLOSE successive integral approximations before the approximations are extrapolated. Used in the resolved resonance calculations. set at .1.

Card type Name	ii	Data Set Entry Name	Entry Description
	4	(i)NCLOSE	Number of times the CLOSE requirement must be met. Used in the resolved resonance calculations. Set at 1.
	5	(i)MXMINI	Maximum number of points to use for any fine or ultra-fine group in resolved resonance integral calculations. Set at 256. If MXMINI is negative.
	6	(i)IUFG	Number of subintervals which the interval about a resonance peak will be broken into in the resolved resonance integral calculations. Set at 1.
	7	WFG	Constant used to determine the energy interval width centered about a resonance peak which will be broken into IUFG ultra-fine groups. Width = WFG/(θ at minimum temperature). θ is described in the resolved resonance calculations, Basic Theory write-up. Set at 1.0.
	8	DIVRG	Divergence criterion used in the resolved resonance integral calculations. Set at 1.001.
DONE			This card type must appear as the last card of any case. It should be placed in back of fixed - format card types described below if they are used.

FLUX CARDS FOLLOW

(fixed-format data-set)

A flux spectra may be input on cards following the above data class header. The formats are the same as for an ENDF/B TAB1 array.

Card 1	Column	Contents	Comment	Format
	1-11	C1	Blank	E11.4
	12-22	C2	Blank	E11.4
	23-33	L1	Blank	I11
	34-44	L2	Blank	I11
	45-55	N1	Number of interpolation "break"points	I11
	56-66	N2	Number of energy-flux points	I11
	67-70	MAT	Material number (Include on all cards)	I4
	71-72	MF	File number (Include on all cards)	I2
	73-75	MT	Reaction number (Include on all cards)	I3
Card 2				
	1-11	NBT(M)	Point at which interpolation scheme ends, i.e. "breakpoint"	I11
	12-22	JNT(M)	Type of interpolation for first range 1 = y constant and equal to value at lower end of the interval 2 = y linear in x 3 = y linear in ln x 4 = ln y linear in x 5 = ln y linear in ln x	I11
		Continue for M = 1,N1		6I11
Card 3				
	1-11	X(N)	Energy point (ev.)	E11.4
	12-22	Y(N)	Flux per unit lethargy at the specified energy point.	E11.4
		Continue for N = 1,N2		6E11.4

UNRESOLVED CARDS FOLLOW

(fixed-format data-set)

If the unresolved resonance cross section contribution has been calculated before for this material with the option for punched cards at each energy point (NDELIF=1 on an UNRESOLVED R card), the cards may be input through this data-set. The presence of these cards will automatically avoid a repeat calculation and will considerably reduce computation time in the unresolved resonance calculations. NOTE: The new case must use the same number of σ_o s and temperatures as the previous case which punched the cards, and the UNRESOLVED R card is still required.

Card 1	Column	Contents	Comment	Format
	1-3	MICT	Number of cross section data sets to follow = (3+LFW)(1+NSGO*NTT).	I3
	4-6	N2	Number of energy points in each data-set.	I3
	7-18	ES(J)	Energy at which cross sections will be given (ev.)	E12.4
		Continue for J = 1,N2		6X,6E12.4
Card 2				
	1-3	N	Card number (1 through MICT) to aid user in ordering.	I3
	4-6	ICT	Output reaction type, all ICT=1 first, then ICT=2,3,4.	I3
	7-18	URXI(ICT,J)	Infinitely dilute, pointwise cross section for reaction type ICT, at energy point J.	E12.4
		Continue for J = 1,N2		6X,6E12.4

Next Card 2 will have:

7-18	URXS(ICT,J,K,L)	Self-shielded, pointwise cross sections for reaction ICT, σ_o(K), temperature(L), at energy point(J).	E12.4
	Continue for J = 1,N2		6X,6E12.4

Vary temperature L first (all temperatures for the same σ_o and ICT), then K, then ICT. Each ICT starts with the infinitely dilute, pointwise cross sections.

ENDF/B FILE FOLLOWS

(fixed-format data-set. If given, it must be the last data set in the deck.)

When running directly from ENDF/B cards, the entire material may be used starting from card 1.

SECTION VI

GLOSSARY OF SYMBOLS

a,b	Parameters for Watt fission spectrum
A	Nuclear mass
a	Channel radius for calculating the penetration factor and energy shift factor = $(1.23A^{1/3}+0.8)\times10^{-1}$
a'	Effective scattering radius for calculating the potential scattering cross section
$(ABN)_c$	Relative abundance which applies to unresolved resonance sequence c.
$(ABN)_{(Is)}$	Relative abundance of isotope Is.
D_c	Average resonance spacing for unresolved sequence c.
E	Neutron Energy
E_{av}	Average energy of fine group
E_c	Energy above which neutron flux spectrum is taken to be a Maxwellian distribution
E_i	Mid-energy of ultrafine group i
E_j	Energy at mid-lethargy of fine group
E_L	Lower energy of group
$E_{L,I}$	Lower energy limit of coarse group I
E_U	Upper energy of group
$E_{o,r}$	Peak energy of resolved resonance r.
$E'_{o,r}$	Effective peak energy of resonance r(corrected for the Phase shift)

E'	Secondary neutron energy in inelastic scattering
f_x	Self-shielding factor for reaction x
$f_{x,n}$	Corrected self-shielding factor for the nth value of σ_o for a given temperature T.
$F(E)$	Function for fine variation of neutron flux with energy
$F_K(E \rightarrow E')$	Fraction of neutrons inelastically scattered at energy E, which have secondary energy E' for Kth distribution
$F_K(E_j \rightarrow E_{j'})$	Fraction of total (n,2n) cross section associated with Kth distribution for initial neutron energy of E_j and final neutron energy of $E_{j'}$
F_ξ	Input parameter for determining which of two methods will be used to calculate the elastic transfer cross sections. Equal to the fraction of the lethargy width of the groups.
g_c	Statistical spin factor for unresolved resonance sequence c
g_x	Multiplying factor for obtaining discrete parameters to represent χ-squared distributions
I	Spin of target nucleus
j	Spin of compound nucleus
k	Neutron wave number = $2.19685(\frac{A}{A+1.0})10^{-3}\sqrt{E}$
K	Boltzman's constant
ℓ	Angular momentum state of incident neutron
N_J	Number of J states in unresolved resonance sequence
N_ℓ	Number of ℓ states in unresolved energy range
N^m	Nuclear density of material m (nuclei/barn-cm)
$(NT)_c$	Contribution to total cross section from all unresolved resonance sequences except sequence c (barns)
$P_{K,j}$	Fraction of total inelastic scattering cross section associated with Kth component, in fine group j
P_ℓ	Penetration factor
$P_q(E)$	Fraction of fission neutron spectrum associated with the qth distribution at energy E.
$S^E_{x,c}$	Parameter distribution correction factor for reaction x and unresolved resonance sequence c at energy E

S_ℓ	Energy shift factor
T	Material temperature
$u_{L,I}$	Lower lethargy of coarse group I
$u_{L,j}$	Lower lethargy of fine group j
$u_{U,I}$	Upper lethargy of coarse group I
$u_{U,j}$	Upper lethargy of fine group j
V_ℓ	Penetration factor for ℓ state
x	Reduced energy displacement from resonance peak energy
y_n	Logarithm of nth value of σ_o for a given temperature
α	Ratio of final to initial neutron energy in maximum energy loss elastic collision
$\langle \Gamma_n^0 \rangle_c^E$	Average reduced neutron width for unresolved resonance sequence c at energy E ($eV^{1/2}$)
Γ_r	Total width for resolved resonance r
Γ_x	Discrete resonance width for reaction x (eV).
$\Gamma_{x,c}^E$	Discrete resonance width for reaction type x and unresolved sequence c at energy E (eV)
$\langle \Gamma_x \rangle_c^E$	Average resonance width for reaction x and unresolved sequence c at energy E (eV)
$\Gamma_{x,r}$	Width for reaction type x for resolved resonance r(eV)
Δ	Doppler width (eV)
ΔE_j	Fine group energy width
Δu_I	Lethargy width of coarse group I
Δu_j	Fine group lethargy width
θ	Discrete level or nuclear temperature for inelastic scattering.
	Nuclear temperature in Maxwellian and fission spectra distributions
λ	Reduced De Broglie wavelength for the neutron

$\lambda_{tr}(E)$	Transport mean free path as a function of energy (cm)
$\langle \lambda_{tr} \rangle_I$	Average transport mean free path for group I (cm)
$\bar{\mu}(E)$	Average cosine of scattering angle for elastic scattering at energy E
$\langle \bar{\mu} \rangle_I$	Average cosine for elastic scattering in coarse group I
$\bar{\mu}_j$	Average cosine for elastic scattering in fine group j
ν	Number of degrees of freedom in χ-squared distribution
$\bar{\nu}(E)$	Average number of neutrons omitted per fission for incident neutron energy E
$\langle \bar{\nu} \rangle_I$	Average number of neutrons produced per fission in coarse group I
ν_j	Average number of neutrons produced per fission in fine group j
ξ	Reduced total resonance width
$\xi(E)$	Average logarithmic energy decrement at energy E
ξ_I	Average logarithmic energy decrement in coarse group I
$\sigma_{er,I}$	Elastic removal cross section in coarse group I
$\sigma_{es,I}$	Elastic scattering cross section in coarse group I
$\sigma_{es}(I \to M)$	Transfer cross section from coarse group I to coarse group M due to elastic scattering
$\sigma_{in,I}$	Total inelastic scattering cross section in coarse group I
$\sigma_{in}(I \to M)$	Inelastic transfer cross section from coarse group I to coarse group M
$\sigma_{in,j}$	Total inelastic scattering cross section in fine group j
$\sigma_{n,2n,I}$	Average (n,2n) cross section for coarse group I
$\sigma_{n,2n}(I \to M)$	Transfer cross section from coarse group I to coarse group M due to (n,2n) reaction

$\sigma_{n,3n,I}$	Average (n,3n) cross section for coarse group I
$\sigma_{p,c}$	Potential scattering for unresolved resonance sequence c (barns)
$\sigma_{P,Ra}$	Potential scattering for resolved resonance range Ra (barns)
$\sigma_{pot}(E)$	Energy dependent potential scattering cross section
σ_{s_j}	Elastic scattering cross section in fine group j (barns)
$\sigma_t^m(E)$	Energy dependent total cross section for material m (barns)
$(\sigma_{x,c}^E)^\infty$	Breit-Wigner infinitely dilute cross section for reaction x and unresolved resonance c, at energy E (barns)
$\sigma_{x,c}^E(\sigma_o,T)$	Cross section for reaction type x due to unresolved resonance sequence c at energy E and for σ_o and temperature T (barns)
$\sigma_{x,c}(\Gamma_{f,k}^*,\Gamma_{n,\ell},T,E')$	Cross section for reaction type x, unresolved resonance sequence c, discrete fission and neutron widths and temperature T at energy E' (barns)
$\sigma_x(E)$	Energy dependent cross section for reaction type x (barns)
$\sigma_{x,i}$	Resolved resonance plus smooth cross section for reaction x for ultrafine group i (barns)
$\sigma_{x,i,h}$	Cross section for reaction x in mini-group h of ultrafine group i (barns)
$\langle \sigma_x^\infty \rangle_I$	Average infinitely dilute cross section in group I for reaction type x (barns)
σ_{x_j}	Interpolated cross section of type x in fine group j (barns)
$\sigma_{x,j}$	Smooth cross section for reaction x for fine group j (barns)
$\sigma_{x,r}(E)$	Cross section for reaction x due to resolved resonance r at energy E (barns)
$\sigma_{x,r}(E_i)$	Cross section for reaction x from resolved resonance r at the ultrafine group energy E_i (barns)

$\langle \sigma_x(\sigma_o) \rangle_I$	Average cross section for reaction type x and σ_o value in group I (barns)
σ_o	Parameter specifying degree of resonance self-shielding (barns)
σ_o^{eff}	Effective resonance self-shielding parameter (barns)
σ_o^I	Value of σ_o at which self-shielding factors are set at 1.0
σ_o^m	Parameter specifying degree of resonance self-shielding for material m (barns)
σ_o^{max}	Maximum value of σ_o input
$\sigma_{o,r}$	Total cross section at unbroadened peak of resonance r (barns)
$\Sigma_t(E)$	Energy dependent macroscopic total cross section (cm^{-1})
$\Sigma_{tr}(E)$	Energy dependent macroscopic transport cross section (cm^{-1})
$\langle \Sigma_{tr} \rangle_I$	Average macroscopic transport cross section for group I (cm^{-1})
$\phi(E)$	Function for coarse variation of neutron flux with energy [$(n/cm^2\text{-sec})$/unit lethargy]
ϕ_j	Fine group neutron flux (n/cm^2-sec)
ϕ_ℓ	Phase shift
ϕ_N	Coarse flux variation normalizing constant
$\Phi(E)$	Total neutron flux as a function of energy [$(n/cm^2\text{-sec}$/unit lethargy]
$\chi(E)$	Spectrum function for neutrons produced by fission
χ_I	Fraction of fission neutrons with energies within coarse group I
$\chi_q(E)$	Fission neutron spectrum for qth distribution at energy E
$\chi(x,\xi)$	Breit-Wigner, Doppler-broadened interference line shape function for reduced parameters x and ξ
$\psi(\chi,\xi)$	Breit-Wigner, Doppler-broadened line shape function for reduced parameters χ and ξ

SECTION VII

SAMPLE PROBLEM

7.1 Description

The input and output listings for a sample problem are given in this section. The listings describe the ENDRUN computations for Pu-239 which is material 1104 on the ENDF/B files. The problem consists of twenty nine groups with resolved, unresolved and smooth contributions to the coarse group cross sections. Self-shielding f-factors were determined, in the resonance range, for one temperature and four discrete values of σ_o.

Downscattering matrix terms were calculated for the (n-2n) and inelastic reactions and an elastic removal cross section was determined for each group.

A standard flux was used for the group weighting functions. That is, above the cutoff energy, E_c, a fission spectrum representation was used and below E_c the flux was assumed to vary as 1/E.

Cards containing the unresolved contribution to the coarse group cross section at thirty energy points were input to bypass the expensive unresolved computations. The cards were generated in a previous problem for the same temperature and σ_o range.

7.2 Output

The output listings for the sample problem include:

a) the input data,

b) intermediate data showing the resonance contribution to the fine groups,

c) coarse group infinitely-dilute cross sections and reaction rates, f-factors and scattering matrices, and

d) a table of computer time.

A GMUG file tape was created in this problem and the size of the data is printed on page 63.

Several pages of the intermediate output have been deleted to conserve space. Enough of this information has been included to indicate the form of the output data.

```
          ENDRUN INPUT DECK

COLUMNS: 12345678901234567890123456789012345678901234567890123456789012345678901234567890
          TITLE          1      ( PU239 MAT, 1104 ENDF/B VERSION 2                        )
           *                    ( 29 GROUPS  TEMPERATURE=300 K  SIGO=10,100,1000,10000    )
           *                    ( RESOLVED  RESONANCE  1-300 EV                           )
           *                    ( UNRESOLVED RESONANCE 300EV-25KEV  30 UNRES,PNTS INPUT   )
          GENERAL        1      1104  2  29  1  29  0.0  2,50  1,41  .5  1104
          OPTIONS        1      0  1  0  0  0
          OUTPUT         1      1  0  0  0  0  2  0  0  0  3  0  0  1
          REACTIONS      1      2 16 18 51,73 102
           *             2      2
           *             3      102
           *             4      18
           *             6      51,73
           *             7      252
           *             8      251
           *             9      16
          DELTA U/CG     1      ,5  1  26   1,5  27  29
          FINE GPS/CG    1      30  1  29
          SIGMA-NOUGHT   1      10,0  100,0  1000,0  10000,0
          TEMPERATURES   1      300,0
          UNRESOLVED R   1      0  2  1  5000,0
           *             5      30  300,0  25000,0  25000,0
           *             9      300, 310, 340, 365, 475, 525, 580, 610, 665, 725,
           *            19      825, 870, 930, 975, 1050, 1075, 1225, 1325,  1550,
           *            28      2000, 2100, 2200, 2400, 2800, 3500, 6500, 8500,
           *            36      10000, 17000, 25000.
          RESOLVED R     1      3  21  29
          MATRIX         1      1  1  1  1  0  15  15  2  1
          UNRESOLVED CARDS FOLLOW     (FROM PREVIOUS CALCULATION)
           20 30  0,3000E 03  0,3100E 03  0,3400E 03  0,3650E 03  0,4750E 03  0,5250E 03
00E 03  0,6100E 03  0,6650E 03  0,7250E 03  0,8250E 03  0,8700E 03
00E 03  0,9750E 03  0,1050E 04  0,1075E 04  0,1225E 04  0,1325E 04
50E 04  0,2000E 04  0,2100E 04  0,2200E 04  0,2400E 04  0,2800E 04
00E 04  0,6500E 04  0,8500E 04  0,1000E 05  0,1700E 05  0,2500E 05
   1  1  0.4099E 02  0,3938E 02  0,3408E 02  0,3101E 02  0,2288E 02  0,4403E 02
40E 02  0,2398E 02  0,2332E 02  0,2308E 02  0,2239E 02  0,2195E 02
18E 02  0,2800E 02  0,2442E 02  0,2190E 02  0,2160E 02  0,2141E 02
00E 02  0,2040E 02  0,2022E 02  0,2001E 02  0,1941E 02  0,1890E 02
09E 02  0,1645E 02  0,1572E 02  0,1505E 02  0,1417E 02  0,1376E 02
   2  1  0,1588E 02  0,1567E 02  0,1530E 02  0,1545E 02  0,1510E 02  0,1758E 02
45E 02  0,1464E 02  0,1463E 02  0,1475E 02  0,1478E 02  0,1472E 02
25E 02  0,1611E 02  0,1554E 02  0,1492E 02  0,1497E 02  0,1529E 02
98E 02  0,1505E 02  0,1502E 02  0,1500E 02  0,1492E 02  0,1498E 02
76E 02  0,1480E 02  0,1452E 02  0,1416E 02  0,1371E 02  0,1348E 02
   3  1  0,2197E 02  0,2152E 02  0,2044E 02  0,2018E 02  0,1836E 02  0,2465E 02
32E 02  0,1821E 02  0,1809E 02  0,1818E 02  0,1806E 02  0,1791E 02
06E 02  0,2069E 02  0,1933E 02  0,1811E 02  0,1810E 02  0,1832E 02
97E 02  0,1786E 02  0,1778E 02  0,1770E 02  0,1743E 02  0,1717E 02
80E 02  0,1593E 02  0,1538E 02  0,1481E 02  0,1407E 02  0,1370E 02
   4  1  0,3461E 02  0,3348E 02  0,3003E 02  0,2811E 02  0,2197E 02  0,3821E 02
13E 02  0,2274E 02  0,2226E 02  0,2212E 02  0,2158E 02  0,2121E 02
46E 02  0,2648E 02  0,2346E 02  0,2123E 02  0,2100E 02  0,2090E 02
51E 02  0,2000E 02  0,1965E 02  0,1956E 02  0,1912E 02  0,1857E 02
91E 02  0,1638E 02  0,1568E 02  0,1502E 02  0,1416E 02  0,1375E 02
   5  1  0,4017E 02  0,3856E 02  0,3355E 02  0,3064E 02  0,2276E 02  0,4331E 02
72E 02  0,2380E 02  0,2320E 02  0,2297E 02  0,2230E 02  0,2187E 02
00E 02  0,2782E 02  0,2430E 02  0,2182E 02  0,2154E 02  0,2135E 02
```

```
0.2095E 02  0.2035E 02  0.2018E 02  0.1997E 02  0.1938E 02  0.1878E 02
0.1807E 02  0.1644E 02  0.1571E 02  0.1504E 02  0.1417E 02  0.1376E 02
                6  2  0.1627E 02  0.1638E 02  0.1488E 02  0.1310E 02  0.1122E 02  0.1805E 02
0.1815E 02  0.1302E 02  0.1295E 02  0.1262E 02  0.1245E 02  0.1243E 02
0.1496E 02  0.1454E 02  0.1323E 02  0.1267E 02  0.1279E 02  0.1210E 02
0.1332E 02  0.1351E 02  0.1386E 02  0.1379E 02  0.1314E 02  0.1276E 02
0.1299E 02  0.1276E 02  0.1226E 02  0.1207E 02  0.1167E 02  0.1152E 02
                7  2  0.1153E 02  0.1157E 02  0.1138E 02  0.1106E 02  0.1065E 02  0.1227E 02
0.1237E 02  0.1127E 02  0.1129E 02  0.1120E 02  0.1119E 02  0.1120E 02
0.1201E 02  0.1192E 02  0.1153E 02  0.1136E 02  0.1146E 02  0.1118E 02
0.1180E 02  0.1201E 02  0.1222E 02  0.1221E 02  0.1191E 02  0.1177E 02
0.1200E 02  0.1220E 02  0.1189E 02  0.1179E 02  0.1153E 02  0.1143E 02
                8  2  0.1284E 02  0.1292E 02  0.1247E 02  0.1175E 02  0.1090E 02  0.1405E 02
0.1421E 02  0.1202E 02  0.1204E 02  0.1186E 02  0.1180E 02  0.1191E 02
0.1327E 02  0.1307E 02  0.1235E 02  0.1203E 02  0.1216E 02  0.1198E 02
0.1264E 02  0.1288E 02  0.1319E 02  0.1315E 02  0.1266E 02  0.1240E 02
0.1265E 02  0.1260E 02  0.1217E 02  0.1200E 02  0.1164E 02  0.1150E 02
                9  2  0.1526E 02  0.1539E 02  0.1426E 02  0.1278E 02  0.1116E 02  0.1700E 02
0.1715E 02  0.1283E 02  0.1279E 02  0.1248E 02  0.1234E 02  0.1233E 02
0.1464E 02  0.1427E 02  0.1308E 02  0.1256E 02  0.1270E 02  0.1204E 02
0.1322E 02  0.1342E 02  0.1377E 02  0.1370E 02  0.1307E 02  0.1271E 02
0.1294E 02  0.1274E 02  0.1225E 02  0.1206E 02  0.1167E 02  0.1152E 02
               10  2  0.1616E 02  0.1625E 02  0.1480E 02  0.1306E 02  0.1121E 02  0.1793E 02
0.1802E 02  0.1299E 02  0.1294E 02  0.1260E 02  0.1244E 02  0.1242E 02
0.1493E 02  0.1451E 02  0.1321E 02  0.1265E 02  0.1278E 02  0.1209E 02
0.1331E 02  0.1350E 02  0.1385E 02  0.1378E 02  0.1313E 02  0.1276E 02
0.1296E 02  0.1275E 02  0.1226E 02  0.1207E 02  0.1167E 02  0.1152E 02
               11  3  0.1373E 02  0.1443E 02  0.1205E 02  0.7567E 01  0.2980E 01  0.9360E 01
0.9112E 01  0.7032E 01  0.6632E 01  0.5324E 01  0.4579E 01  0.4484E 01
0.5800E 01  0.5368E 01  0.4258E 01  0.4109E 01  0.3948E 01  0.2571E 01
0.4166E 01  0.3751E 01  0.4175E 01  0.3992E 01  0.3076E 01  0.2441E 01
0.2445E 01  0.1685E 01  0.1197E 01  0.1100E 01  0.7087E 00  0.5501E 00
               12  3  0.3939E 01  0.4221E 01  0.3904E 01  0.2702E 01  0.1390E 01  0.3163E 01
0.3201E 01  0.3199E 01  0.3127E 01  0.2586E 01  0.2331E 01  0.2331E 01
0.2691E 01  0.2563E 01  0.2198E 01  0.2235E 01  0.2218E 01  0.1494E 01
0.2481E 01  0.2370E 01  0.2682E 01  0.2595E 01  0.2047E 01  0.1689E 01
0.1778E 01  0.1448E 01  0.1063E 01  0.9997E 00  0.6704E 00  0.5307E 00
               13  3  0.7187E 01  0.7673E 01  0.6910E 01  0.4621E 01  0.2164E 01  0.5418E 01
0.5423E 01  0.5074E 01  0.4893E 01  0.3991E 01  0.3527E 01  0.3498E 01
0.4191E 01  0.3950E 01  0.3291E 01  0.3283E 01  0.3209F 01  0.2120E 01
0.3493E 01  0.3233E 01  0.3628E 01  0.3457E 01  0.2714E 01  0.2190E 01
0.2239E 01  0.1623E 01  0.1165E 01  0.1078E 01  0.7005F 00  0.5463E 00
               14  3  0.1204E 02  0.1269E 02  0.1084E 02  0.6912E 01  0.2825E 01  0.8432E 01
0.8261E 01  0.6684E 01  0.6334E 01  0.5098E 01  0.4407E 01  0.4327E 01
0.5516E 01  0.5121F 01  0.4099F 01  0.3981E 01  0.3836F 01  0.2501E 01
0.4073E 01  0.3677E 01  0.4101E 01  0.3922E 01  0.3024F 01  0.2406E 01
0.2418E 01  0.1675E 01  0.1192E 01  0.1097E 01  0.7070F 00  0.5494E 00
               15  3  0.1356E 02  0.1421E 02  0.1190E 02  0.7477E 01  0.2950E 01  0.9264E 01
0.9009E 01  0.6988E 01  0.6598E 01  0.5295E 01  0.4558E 01  0.4467E 01
0.5772E 01  0.5340E 01  0.4238E 01  0.4094E 01  0.3935E 01  0.2560E 01
0.4161E 01  0.3742E 01  0.4168E 01  0.3994E 01  0.3067E 01  0.2435E 01
0.2442E 01  0.1682E 01  0.1195E 01  0.1100E 01  0.7078E 00  0.5498E 00
               16  4  0.1098E 02  0.8576E 01  0.7144E 01  0.1034E 02  0.8676E 01  0.1662E 02
0.1514E 02  0.3924E 01  0.3731E 01  0.5140E 01  0.5360E 01  0.5036E 01
0.8429E 01  0.8082E 01  0.6925E 01  0.5123E 01  0.4861E 01  0.6731E 01
0.3520E 01  0.3137E 01  0.2181E 01  0.2230E 01  0.3198E 01  0.3599E 01
0.2659E 01  0.2010E 01  0.2260E 01  0.1879E 01  0.1795E 01  0.1694E 01
               17  4  0.5043E 01  0.4301E 01  0.3782E 01  0.5055E 01  0.5141E 01  0.7528E 01
0.7065E 01  0.2516E 01  0.2448E 01  0.3135E 01  0.3326E 01  0.3179E 01
0.4793E 01  0.4675E 01  0.4224E 01  0.3300E 01  0.3206E 01  0.4447E 01
```

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0.2501E 01  0.2332E 01  0.1742E 01  0.1778E 01  0.2419E 01  0.2733E 01
0.2137E 01  0.1792E 01  0.2051E 01  0.1743E 01  0.1718E 01  0.1646E 01
                18  4  0.7454E 01  0.6157E 01  0.5330E 01  0.7424E 01  0.7072E 01  0.1124E 02
0.1044E 02  0.3296E 01  0.3186E 01  0.4262E 01  0.4482E 01  0.4230E 01
0.6675E 01  0.6473E 01  0.5740E 01  0.4373E 01  0.4202E 01  0.5847E 01
0.3140E 01  0.2860E 01  0.2042E 01  0.2089E 01  0.2946E 01  0.3326E 01
0.2505E 01  0.1956E 01  0.2212E 01  0.1849E 01  0.1780E 01  0.1695E 01
                19  4  0.1017E 02  0.8043E 01  0.6775E 01  0.9761E 01  0.8415E 01  0.1545E 02
0.1414E 02  0.3801E 01  0.3646E 01  0.5004E 01  0.5225E 01  0.4915E 01
0.8137E 01  0.7814E 01  0.6739E 01  0.5007E 01  0.4764E 01  0.6609E 01
0.3458E 01  0.3098E 01  0.2161E 01  0.2211E 01  0.3167E 01  0.3565E 01
0.2637E 01  0.2002E 01  0.2255E 01  0.1875E 01  0.1793E 01  0.1693E 01
                20  4  0.1089E 02  0.8506E 01  0.7099E 01  0.1028E 02  0.8645E 01  0.1650E 02
0.1502E 02  0.3886E 01  0.3722E 01  0.5129E 01  0.5346E 01  0.5022E 01
0.8403E 01  0.8051E 01  0.6903E 01  0.5106E 01  0.4850E 01  0.6723E 01
0.3504E 01  0.3132E 01  0.2177E 01  0.2228E 01  0.3198E 01  0.3597E 01
0.2654E 01  0.2008E 01  0.2260E 01  0.1878E 01  0.1795E 01  0.1694E 01
                DONE
CARD COLUMNS: 12345678901234567890123456789012345678901234567890123456789012345678901234567890
```

ENDRUN INPUT EDIT

ENDRUN INPUT EDIT

CROSS-SECTION CONTRIBUTION

	COARSE GROUP	HIGHEST LETHARGY	LOWEST ENERGY	NUMBER OF FINE GROUPS	SMOOTH	RESOLVED RESONANCE	UNRESOLVED RESONANCE
		0.	1.000E 07				
IMIN	1	5.000E-01	6.065E 06	30	INF-DIL	NONE	NONE
	2	1.000E 00	3.679E 06	30	INF-DIL	NONE	NONE
	3	1.500E 00	2.231E 06	30	INF-DIL	NONE	NONE
	4	2.000E 00	1.353E 06	30	INF-DIL	NONE	NONE
	5	2.500E 00	8.208E 05	30	INF-DIL	NONE	NONE
	6	3.000E 00	4.979E 05	30	INF-DIL	NONE	NONE
	7	3.500E 00	3.020E 05	30	INF-DIL	NONE	NONE
	8	4.000E 00	1.832E 05	30	INF-DIL	NONE	NONE
	9	4.500E 00	1.111E 05	30	INF-DIL	NONE	NONE
	10	5.000E 00	6.738E 04	30	INF-DIL	NONE	NONE
	11	5.500E 00	4.087E 04	30	INF-DIL	NONE	NONE
	12	6.000E 00	2.479E 04	30	INF-DIL	NONE	F-FACTR
	13	6.500E 00	1.503E 04	30	INF-DIL	NONE	F-FACTR
	14	7.000E 00	9.119E 03	30	INF-DIL	NONE	F-FACTR
	15	7.500E 00	5.531E 03	30	INF-DIL	NONE	F-FACTR
	16	8.000E 00	3.355E 03	30	INF-DIL	NONE	F-FACTR
	17	8.500E 00	2.035E 03	30	INF-DIL	NONE	F-FACTR
	18	9.000E 00	1.234E 03	30	INF-DIL	NONE	F-FACTR
	19	9.500E 00	7.485E 02	30	INF-DIL	NONE	F-FACTR
	20	1.000E 01	4.540E 02	30	INF-DIL	NONE	F-FACTR
	21	1.050E 01	2.754E 02	30	INF-DIL	F-FACTR	F-FACTR
	22	1.100E 01	1.670E 02	30	INF-DIL	F-FACTR	NONE
	23	1.150E 01	1.013E 02	30	INF-DIL	F-FACTR	NONE
	24	1.200E 01	6.144E 01	30	INF-DIL	F-FACTR	NONE
	25	1.250E 01	3.727E 01	30	INF-DIL	F-FACTR	NONE
	26	1.300E 01	2.260E 01	30	INF-DIL	F-FACTR	NONE
	27	1.450E 01	5.043E 00	30	INF-DIL	F-FACTR	NONE
	28	1.600E 01	1.125E 00	30	INF-DIL	F-FACTR	NONE
IMAX	29	1.750E 01	2.511E-01	30	INF-DIL	F-FACTR	NONE

F-FACTOR SIGMA-NOUGHT VALUES: 1.000E 01, 1.000E 02, 1.000E 03, 1.000E 04

F-FACTOR TEMPERATURES: 3.000E 02

ENDF/B DATA WILL BE READ FROM NPOST TAPE

ENDF/B MT VALUES INCLUDED IN ENDRUN TOTAL REACTION (ICT = 1): 2, 16, 18, 51, 73,102
SCAT (ICT = 2): 2
CAP (ICT = 3): 102
FISS (ICT = 4): 18
INELAS (ICT = 6): 51, 73
XI (ICT = 7): 252
MU (ICT = 8): 251
N-2N (ICT = 9): 16

U HAS BEEN READ AND WRITTEN ON DISC FOR LATER USE

)ENDR CASE ID NO, PU239 CASE SEQUENCE NO, 1 050771 0326,1 PAGE NO, 3

UNRESOLVED CONTRIBUTION TO TOTAL CROSS-SECTION

GROUP	INF DILUTE	TEMP	SIG-O 10,0	100,0	1000,0	10000,0
12	4,58674E-01	300,	4,49337E-01	4,56673E-01	4,58340E-01	4,58674E-01
13	1,40424E 01	300,	1,36376E 01	1,39535E 01	1,40319E 01	1,40421E 01
14	1,48047E 01	300,	1,40365E 01	1,46046E 01	1,47806E 01	1,47979E 01
15	1,61958E 01	300,	1,46726E 01	1,57226E 01	1,61342E 01	1,61854E 01
16	1,75275E 01	300,	1,47745E 01	1,65047E 01	1,73860E 01	1,75110E 01
17	1,91626E 01	300,	1,49041E 01	1,73175E 01	1,88937E 01	1,91351E 01
18	2,09592E 01	300,	1,50719E 01	1,80280E 01	2,04839E 01	2,09063E 01
19	2,38177E 01	300,	1,52208E 01	1,88418E 01	2,28600E 01	2,37100E 01
20	3,00216E 01	300,	1,57439E 01	2,03835E 01	2,74963E 01	2,97036E 01
21	2,61792E 01	300,	1,28302E 01	1,67569E 01	2,34756E 01	2,58258E 01

UNRESOLVED CONTRIBUTION TO SCAT CROSS-SECTION

INF DILUTE	TEMP	SIG0			
		10.0	100.0	1000.0	10000.0
3.84003E-01	300.	3.81002E-01	3.83336E-01	3.84003E-01	3.84003E-01
1.16258E 01	300.	1.15004E 01	1.15984E 01	1.16255E 01	1.16258E 01
1.19535E 01	300.	1.17133E 01	1.18952E 01	1.19467E 01	1.19535E 01
1.25585E 01	300.	1.20614E 01	1.24205E 01	1.25414E 01	1.25527E 01
1.29101E 01	300.	1.20655E 01	1.26311E 01	1.28703E 01	1.29001E 01
1.31356E 01	300.	1.19410E 01	1.26793E 01	1.30711E 01	1.31293E 01
1.30529E 01	300.	1.16935E 01	1.24528E 01	1.29661E 01	1.30429E 01
1.31518E 01	300.	1.14717E 01	1.22660E 01	1.29976E 01	1.31339E 01
1.43234E 01	300.	1.15080E 01	1.25096E 01	1.38928E 01	1.42710E 01
1.13805E 01	300.	9.27558E 00	9.93977E 00	1.10075E 01	1.13328E 01

)ENDR CASE ID NO. PU239 CASE SEQUENCE NO. 1 050771 0326,1 PAGE NO. 5

UNRESOLVED CONTRIBUTION TO CAP CROSS-SECTION

GROUP	INF DILUTE	TEMP	SIG0 10.0	100.0	1000.0	10000.0
12	1.83391E-02	300.	1.76922E-02	1.82124E-02	1.83158E-02	1.83291E-02
13	6.56800E-01	300.	6.24644E-01	6.50052E-01	6.55468E-01	6.56154E-01
14	9.69146E-01	300.	8.89689E-01	9.51686E-01	9.66508E-01	9.68697E-01
15	1.50231E 00	300.	1.29609E 00	1.44889E 00	1.49398E 00	1.49980E 00
16	2.16358E 00	300.	1.65987E 00	2.01323E 00	2.14314E 00	2.16052E 00
17	2.97596E 00	300.	2.00794E 00	2.64049E 00	2.92929E 00	2.96927E 00
18	3.63050E 00	300.	2.18517E 00	3.05501E 00	3.54764E 00	3.62218E 00
19	4.65153E 00	300.	2.37267E 00	3.57322E 00	4.47354E 00	4.63108E 00
20	6.59931E 00	300.	2.72260E 00	4.40390E 00	6.14315E 00	6.54399E 00
21	7.09628E 00	300.	2.40670E 00	4.17180E 00	6.46618E 00	7.00632E 00

)ENDR CASE ID NO. PU239 CASE SEQUENCE NO. 1 050771 0326,1 PAGE NO. 6

UNRESOLVED CONTRIBUTION TO FISS CROSS-SECTION

GROUP	INF DILUTE	TEMP	SIGO			
			10.0	100.0	1000.0	10000.0
12	5.64684E-02	300.	5.48679E-02	5.61683E-02	5.64350E-02	5.64684E-02
13	1.75973E 00	300.	1.69196E 00	1.74657E 00	1.75805E 00	1.75970E 00
14	1.87108E 00	300.	1.75035E 00	1.84502E 00	1.86767E 00	1.87044E 00
15	2.12281E 00	300.	1.89990E 00	2.06832E 00	2.11555E 00	2.12147E 00
16	2.43031E 00	300.	2.01928E 00	2.31331E 00	2.41354E 00	2.42646E 00
17	3.02760E 00	300.	2.33583E 00	2.80963E 00	2.99954E 00	3.02532E 00
18	4.17875E 00	300.	2.91540E 00	3.70526E 00	4.10852E 00	4.16779E 00
19	6.00358E 00	300.	3.68359E 00	4.97927E 00	5.84147E 00	5.98569E 00
20	8.99433E 00	300.	4.72670E 00	6.69991E 00	8.53463E 00	8.94003E 00
21	7.56190E 00	300.	3.91843E 00	5.61019E 00	7.17448E 00	7.51777E 00

UNRESOLVED RESONANCE INFINITELY DILUTE FINE GROUP CROSS SECTIONS
CROSS SECTIONS

COARSE GROUP	FINE GROUP	HIGHEST ENERGY	TOTAL	SCATTER	CAPTURE	FISSION
12	1	2,499E 04	1,376E 01	1,152E 01	5,502E-01	1,694E 00
	2	2,542E 04	0.	0.	0.	0.
	3	2,584E 04	0.	0.	0.	0.
	4	2,628E 04	0.	0.	0.	0.
	5	2,672E 04	0.	0.	0.	0.
	6	2,717E 04	0.	0.	0.	0.
	7	2,762E 04	0.	0.	0.	0.
	8	2,809E 04	0.	0.	0.	0.
	9	2,856E 04	0.	0.	0.	0.
	10	2,904E 04	0.	0.	0.	0.
	11	2,953E 04	0.	0.	0.	0.
	12	3,002E 04	0.	0.	0.	0.
	13	3,053E 04	0.	0.	0.	0.
	14	3,104E 04	0.	0.	0.	0.
	15	3,156E 04	0.	0.	0.	0.
	16	3,209E 04	0.	0.	0.	0.
	17	3,263E 04	0.	0.	0.	0.
	18	3,318E 04	0.	0.	0.	0.
	19	3,374E 04	0.	0.	0.	0.
	20	3,431E 04	0.	0.	0.	0.
	21	3,488E 04	0.	0.	0.	0.
	22	3,547E 04	0.	0.	0.	0.
	23	3,607E 04	0.	0.	0.	0.
	24	3,667E 04	0.	0.	0.	0.
	25	3,729E 04	0.	0.	0.	0.
	26	3,791E 04	0.	0.	0.	0.
	27	3,855E 04	0.	0.	0.	0.
	28	3,920E 04	0.	0.	0.	0.
	29	3,986E 04	0.	0.	0.	0.
	30	4,053E 04	0.	0.	0.	0.
13	1	1,516E 04	1,436E 01	1,176E 01	7,792E-01	1,813E 00
	2	1,541E 04	1,433E 01	1,174E 01	7,686E-01	1,810E 00
	3	1,567E 04	1,430E 01	1,173E 01	7,580E-01	1,808E 00
	4	1,594E 04	1,427E 01	1,172E 01	7,476E-01	1,805E 00
	5	1,621E 04	1,425E 01	1,171E 01	7,374E-01	1,802E 00
	6	1,648E 04	1,422E 01	1,169E 01	7,273E-01	1,800E 00
	7	1,675E 04	1,419E 01	1,168E 01	7,173E-01	1,797E 00
	8	1,704E 04	1,417E 01	1,167E 01	7,077E-01	1,794E 00
	9	1,732E 04	1,415E 01	1,166E 01	7,000E-01	1,790E 00
	10	1,761E 04	1,413E 01	1,166E 01	6,924E-01	1,785E 00
	11	1,791E 04	1,411E 01	1,165E 01	6,848E-01	1,781E 00
	12	1,821E 04	1,410E 01	1,164E 01	6,774E-01	1,777E 00
	13	1,852E 04	1,408E 01	1,164E 01	6,700E-01	1,772E 00
	14	1,883E 04	1,406E 01	1,163E 01	6,627E-01	1,768E 00
	15	1,914E 04	1,404E 01	1,162E 01	6,555E-01	1,763E 00
	16	1,947E 04	1,402E 01	1,162E 01	6,484E-01	1,759E 00
	17	1,979E 04	1,401E 01	1,161E 01	6,413E-01	1,754E 00
	18	2,013E 04	1,399E 01	1,160E 01	6,343E-01	1,750E 00
	19	2,046E 04	1,397E 01	1,160E 01	6,274E-01	1,746E 00
	20	2,081E 04	1,395E 01	1,159E 01	6,206E-01	1,741E 00
	21	2,116E 04	1,394E 01	1,158E 01	6,138E-01	1,737E 00

UNRESOLVED RESONANCE INFINITELY DILUTE FINE GROUP CROSS SECTIONS

CROSS SECTIONS

NE UP	HIGHEST ENERGY	TOTAL	SCATTER	CAPTURE	FISSION
2	2.151E 04	1.392E 01	1.158E 01	6.071E-01	1.733E 00
3	2.187E 04	1.390E 01	1.157E 01	6.005E-01	1.728E 00
4	2.224E 04	1.388E 01	1.157E 01	5.940E-01	1.724E 00
5	2.262E 04	1.387E 01	1.156E 01	5.875E-01	1.720E 00
6	2.300E 04	1.385E 01	1.155E 01	5.811E-01	1.715E 00
7	2.338E 04	1.383E 01	1.155E 01	5.748E-01	1.711E 00
8	2.378E 04	1.381E 01	1.154E 01	5.685E-01	1.707E 00
9	2.418E 04	1.380E 01	1.153E 01	5.624E-01	1.703E 00
0	2.458E 04	1.378E 01	1.153E 01	5.562E-01	1.698E 00
1	9.195E 03	1.539E 01	1.217E 01	1.149E 00	2.067E 00
2	9.350E 03	1.532E 01	1.215E 01	1.139E 00	2.028E 00
3	9.507E 03	1.526E 01	1.213E 01	1.129E 00	1.990E 00
4	9.667E 03	1.519E 01	1.211E 01	1.120E 00	1.953E 00
5	9.829E 03	1.512E 01	1.209E 01	1.110E 00	1.916E 00
6	9.994E 03	1.505E 01	1.207E 01	1.100E 00	1.880E 00
7	1.016E 04	1.502E 01	1.206E 01	1.085E 00	1.876E 00
8	1.033E 04	1.499E 01	1.204E 01	1.071E 00	1.874E 00
9	1.051E 04	1.497E 01	1.203E 01	1.056E 00	1.871E 00
0	1.068E 04	1.494E 01	1.202E 01	1.041E 00	1.868E 00
1	1.086E 04	1.491E 01	1.201E 01	1.027E 00	1.866E 00
2	1.105E 04	1.488E 01	1.199E 01	1.013E 00	1.863E 00
3	1.123E 04	1.485E 01	1.198E 01	9.991E-01	1.860E 00
4	1.142E 04	1.482E 01	1.197E 01	9.854E-01	1.858E 00
5	1.161E 04	1.480E 01	1.196E 01	9.719E-01	1.855E 00
6	1.181E 04	1.477E 01	1.194E 01	9.586E-01	1.852E 00
7	1.201E 04	1.474E 01	1.193E 01	9.454E-01	1.850E 00
8	1.221E 04	1.471E 01	1.192E 01	9.325E-01	1.847E 00
9	1.241E 04	1.469E 01	1.191E 01	9.197E-01	1.844E 00
0	1.262E 04	1.466E 01	1.189E 01	9.071E-01	1.842E 00
1	1.283E 04	1.463E 01	1.188E 01	8.946E-01	1.839E 00
2	1.305E 04	1.460E 01	1.187E 01	8.824E-01	1.836E 00
3	1.327E 04	1.457E 01	1.186E 01	8.703E-01	1.834E 00
4	1.349E 04	1.455E 01	1.184E 01	8.583E-01	1.831E 00
5	1.372E 04	1.452E 01	1.183E 01	8.466E-01	1.829E 00
6	1.395E 04	1.449E 01	1.182E 01	8.350E-01	1.826E 00
7	1.418E 04	1.446E 01	1.181E 01	8.235E-01	1.823E 00
8	1.442E 04	1.444E 01	1.179E 01	8.122E-01	1.821E 00
9	1.466E 04	1.441E 01	1.178E 01	8.011E-01	1.818E 00
1	1.491E 04	1.438E 01	1.177E 01	7.901E-01	1.815E 00
	5.577E 03	1.684E 01	1.282E 01	1.848E 00	2.154E 00
	5.671E 03	1.680E 01	1.281E 01	1.829E 00	2.138E 00
	5.766E 03	1.676E 01	1.280E 01	1.811E 00	2.122E 00
	5.863E 03	1.671E 01	1.280E 01	1.793E 00	2.106E 00
	5.962E 03	1.667E 01	1.279E 01	1.775E 00	2.090E 00
	6.062E 03	1.663E 01	1.279E 01	1.757E 00	2.074E 00
	6.164E 03	1.658E 01	1.278E 01	1.740E 00	2.059E 00
	6.267E 03	1.654E 01	1.277E 01	1.722E 00	2.043E 00
	6.373E 03	1.650E 01	1.277E 01	1.705E 00	2.028E 00
	6.480E 03	1.646E 01	1.276E 01	1.688E 00	2.013E 00
	6.589E 03	1.641E 01	1.273E 01	1.656E 00	2.022E 00

Pages 9 through 12 have been deleted to conserve space.

LUS RESOLVED RESONANCE FINE GROUP CROSS SECTIONS

FINE GROUP	LOWEST LETHARGY	HIGHEST ENERGY	TEMP	SIGMA-NOUGHT	CROSS-SECTIONS TOTAL	SCATTER	CAPTURE	FISSION
1	.1000E 02	.4540E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
2	.1002E 02	.4465E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
3	.1003E 02	.4391E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
4	.1005E 02	.4319E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
5	.1007E 02	.4247E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
6	.1008E 02	.4177E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
7	.1010E 02	.4108E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				
8	.1012E 02	.4040E 03		INF-DIL				
			300.	10.				
				100.				
				1000.				
				10000.				

SMOOTH PLUS RESOLVED RESONANCE FINE GROUP CROSS SECTIONS ,PAGE 2

COARSE GROUP	FINE GROUP	LOWEST LETHARGY	HIGHEST ENERGY	TEMP	SIGMA-NOUGHT	CROSS-SECTIONS TOTAL	SCATTER	CAPTURE	FISSION
21	9	.1013E 02	.3973E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	10	.1015E 02	.3908E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	11	.1017E 02	.3843E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	12	.1018E 02	.3780E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	13	.1020E 02	.3717E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	14	.1022E 02	.3656E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	15	.1023E 02	.3595E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	16	.1025E 02	.3536E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				

SMOOTH PLUS RESOLVED RESONANCE FINE GROUP CROSS SECTIONS ,PAGE 3

COARSE GROUP	FINE GROUP	LOWEST LETHARGY	HIGHEST ENERGY	TEMP	SIGMA-NOUGHT	CROSS-SECTIONS TOTAL	SCATTER	CAPTURE	FISSION
21	17	.1027E 02	,3477E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	18	.1028E 02	,3420E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	19	.1030E 02	,3363E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	20	.1032E 02	,3308E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	21	.1033E 02	,3253E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	22	.1035E 02	,3199E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	23	.1037E 02	,3146E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				
	24	.1038E 02	,3094E 03	300.	INF-DIL				
					10.				
					100.				
					1000.				
					10000.				

RESOLVED RESONANCE FINE GROUP CROSS SECTIONS ,PAGE 4

E LOWEST P LETHARGY	HIGHEST ENERGY	TEMP	SIGMA-NOUGHT	CROSS-SECTIONS TOTAL	SCATTER	CAPTURE	FISSION
.1040E 02	,3043E 03		INF-DIL	,1929E 01	,1799E 01	,4234E-01	,8683E-01
		300.	10.	,1200E 01	,1425E 01	,3348E-01	,6869E-01
			100.	,1607E 01	,1644E 01	,3866E-01	,7929E-01
			1000.	,1880E 01	,1777E 01	,4180E-01	,8573E-01
			10000.	,1923E 01	,1797E 01	,4229E-01	,8672E-01
.1042E 02	,2993E 03		INF-DIL	,4519E 02	,1475E 02	,1081E 02	,1963E 02
		300.	10.	,2576E 02	,1327E 02	,5447E 01	,1280E 02
			100.	,3333E 02	,1396E 02	,7990E 01	,1616E 02
			1000.	,4265E 02	,1460E 02	,1028E 02	,1899E 02
			10000.	,4490E 02	,1473E 02	,1075E 02	,1956E 02
.1043E 02	,2943E 03		INF-DIL	,2834E 02	,1301E 02	,1636E 01	,1370E 02
		300.	10.	,2284E 02	,1286E 02	,1265E 01	,1077E 02
			100.	,2558E 02	,1295E 02	,1493E 01	,1257E 02
			1000.	,2797E 02	,1300E 02	,1616E 01	,1354E 02
			10000.	,2830E 02	,1301E 02	,1634E 01	,1368E 02
.1045E 02	,2895E 03		INF-DIL	,2034E 02	,1395E 02	,6739E 00	,5717E 01
		300.	10.	,2029E 02	,1393E 02	,6718E 00	,5717E 01
			100.	,2033E 02	,1394E 02	,6734E 00	,5717E 01
			1000.	,2034E 02	,1395E 02	,6738E 00	,5717E 01
			10000.	,2034E 02	,1395E 02	,6739E 00	,5717E 01
.1047E 02	,2847E 03		INF-DIL	,7578E 02	,3324E 02	,3211E 02	,1043E 02
		300.	10.	,2442E 02	,1756E 02	,7473E 01	,7101E 01
			100.	,3237E 02	,2220E 02	,1452E 02	,8042E 01
			1000.	,5973E 02	,3014E 02	,2713E 02	,9751E 01
			10000.	,7362E 02	,3286E 02	,3149E 02	,1034E 02
.1048E 02	,2800E 03		INF-DIL	,6378E 02	,1935E 02	,1409E 02	,3035E 02
		300.	10.	,3191E 02	,1634E 02	,7071E 01	,1701E 02
			100.	,4162E 02	,1765E 02	,1020E 02	,2223E 02
			1000.	,5822E 02	,1900E 02	,1335E 02	,2853E 02
			10000.	,6312E 02	,1931E 02	,1400E 02	,3014E 02
.1050E 02	,2754E 03		INF-DIL	,1209E 03	,3024E 02	,3478E 02	,5584E 02
		300.	10.	,3311E 02	,1498E 02	,1124E 02	,2510E 02
			100.	,5016E 02	,1976E 02	,1833E 02	,3523E 02
			1000.	,9679E 02	,2733E 02	,3015E 02	,5055E 02
			10000.	,1177E 03	,2988E 02	,3421E 02	,5520E 02
.1052E 02	,2706E 03		INF-DIL	,3558E 02	,1000E 02	,2172E 01	,2341E 02
		300.	10.	,2836E 02	,9784E 01	,1713E 01	,1954E 02
			100.	,3202E 02	,9909E 01	,1974E 01	,2175E 02
			1000.	,3500E 02	,9988E 01	,2142E 01	,2316E 02
			10000.	,3552E 02	,1000E 02	,2168E 01	,2338E 02

Pages 17 through 46 have been deleted to conserve space.

SMOOTH PLUS RESOLVED RESONANCE CONTRIBUTION TO TOTAL CROSS-SECTION

GROUP	INF DILUTE	TEMP	SIG-O 10.0	100.0	1000.0	10000.0
21	7.84546E 00	300.	4.84067E 00	4.92623E 00	6.81875E 00	7.70804E 00
22	4.02618E 01	300.	1.87866E 01	2.49472E 01	3.55101E 01	3.96432E 01
23	5.22962E 01	300.	1.80270E 01	2.57632E 01	4.15754E 01	5.06147E 01
24	7.78804E 01	300.	2.20892E 01	3.02895E 01	4.88398E 01	7.09717E 01
25	1.22029E 02	300.	1.53179E 01	2.85183E 01	6.90713E 01	1.10527E 02
26	4.04577E 01	300.	1.29184E 01	1.77324E 01	2.97314E 01	3.86893E 01
27	1.40038E 02	300.	2.21206E 01	3.19647E 01	7.03676E 01	1.23769E 02
28	2.99124E 01	300.	2.59675E 01	2.84843E 01	2.97176E 01	2.98922E 01
29	1.25612E 03	300.	9.10690E 01	1.14893E 02	2.66872E 02	8.46987E 02

SMOOTH PLUS RESOLVED RESONANCE CONTRIBUTION TO SCAT CROSS-SECTION

GROUP	INF DILUTE	TEMP	SIGO			
			10.0	100.0	1000.0	10000.0
21	3.20337E 00	300.	2.58640E 00	2.64499E 00	3.03723E 00	3.18249E 00
22	1.37136E 01	300.	1.13715E 01	1.21555E 01	1.32834E 01	1.36598E 01
23	1.44124E 01	300.	1.08443E 01	1.17162E 01	1.33940E 01	1.42603E 01
24	1.65426E 01	300.	1.14647E 01	1.22329E 01	1.42358E 01	1.60874E 01
25	1.79360E 01	300.	8.18861E 00	9.89487E 00	1.38253E 01	1.71473E 01
26	9.52972E 00	300.	8.93131E 00	9.14077E 00	9.39200E 00	9.50982E 00
27	1.09325E 01	300.	9.12707E 00	9.42567E 00	1.01697E 01	1.07848E 01
28	1.04200E 01	300.	1.02923E 01	1.03786E 01	1.04146E 01	1.04194E 01
29	1.33602E 01	300.	1.21468E 01	1.23434E 01	1.28464E 01	1.32552E 01

)ENDR CASE ID NO. PU239 CASE SEQUENCE NO. 1 050771 0326,1 PAGE NO. 49

SMOOTH PLUS RESOLVED RESONANCE CONTRIBUTION TO CAP SIGMA CROSS-SECTION

GROUP	INF DILUTE	TEMP	10.0	100.0	1000.0	10000.0
21	1.97859E 00	300.	6.85709E-01	1.07203E 00	1.72693E 00	1.94723E 00
22	8.75791E 00	300.	2.86619E 00	5.06254E 00	7.83243E 00	8.64528E 00
23	1.58132E 01	300.	3.97791E 00	7.43236E 00	1.30340E 01	1.54221E 01
24	1.55653E 01	300.	2.77431E 00	5.10545E 00	1.05641E 01	1.46225E 01
25	5.79645E 01	300.	7.30630E 00	1.52036E 01	3.63712E 01	5.39074E 01
26	1.59325E 01	300.	3.46614E 00	6.85201E 00	1.27078E 01	1.54715E 01
27	5.10735E 01	300.	7.25770E 00	1.36937E 01	3.18672E 01	4.73882E 01
28	3.64314E 00	300.	3.02582E 00	3.42868E 00	3.61438E 00	3.64016E 00
29	4.93335E 02	300.	5.62054E 01	8.00384E 01	1.93840E 02	4.00847E 02

SMOOTH PLUS RESOLVED RESONANCE CONTRIBUTION TO FISS CROSS-SECTION

INF DILUTE	TEMP	SIGZO 10,0	100,0	1000,0	10000,0
2,66349E 00	300,	1,77256E 00	2,05680E 00	2,51751E 00	2,64621E 00
1,77902E 01	300,	9,04279E 00	1,26574E 01	1,65655E 01	1,76442E 01
2,20706E 01	300,	9,04780E 00	1,38369E 01	1,96932E 01	2,17548E 01
4,57725E 01	300,	1,48354E 01	2,16092E 01	3,40227E 01	4,35283E 01
4,61285E 01	300,	1,08664E 01	2,20911E 01	3,83091E 01	4,49603E 01
1,49955E 01	300,	3,90317E 00	6,81868E 00	1,20377E 01	1,45711E 01
7,80323E 01	300,	1,58940E 01	2,64923E 01	5,27391E 01	7,33226E 01
1,58493E 01	300,	1,44109E 01	1,53679E 01	1,57856E 01	1,58427E 01
7,49430E 02	300,	1,08764E 02	1,46500E 02	3,17083E 02	6,16711E 02

1.3580E 01	0.
1.4208E 01	0.
1.4843E 01	0.
1.6197E 01	0.
1.7528E 01	0.
1.9163E 01	0.
2.0959E 01	0.
2.3818E 01	0.
3.0022E 01	0.
3.4025E 01	0.
4.0262E 01	0.
5.2296E 01	0.
7.7880E 01	0.
1.2203E 02	0.
4.0458E 01	0.
1.4004E 02	0.
2.9912E 01	0.
1.2561E 03	0.

DIFFERENCE OF 7.2071E-04 BETWEEN SIG-INELAS AND SUM OF MATRIX FROM SOURCE GROUP 2 WAS SPREAD OVER WHOLE M
DIFFERENCE OF 5.8569E-03 BETWEEN SIG-INELAS AND SUM OF MATRIX FROM SOURCE GROUP 3 WAS SPREAD OVER WHOLE M
DIFFERENCE OF 2.6552E-02 BETWEEN SIG-INELAS AND SUM OF MATRIX FROM SOURCE GROUP 4 WAS SPREAD OVER WHOLE M
DIFFERENCE OF 1.8994E-02 BETWEEN SIG-INELAS AND SUM OF MATRIX FROM SOURCE GROUP 5 WAS SPREAD OVER WHOLE M

INFINITELY DILUTE COARSE GROUP AVERAGE CROSS SECTIONS

TOTAL-SUM	ELASTIC	CAPTURE	FISSION	TOTAL	INELASTIC	LETHARGY GAIN
6.68678E 00	3.15599E 00	1.30684E-03	2.03969E 00	0.	1.40950E 00	1.
7.80968E 00	3.92414E 00	2.62394E-03	1.71043E 00	0.	2.17220E 00	1.
7.80143E 00	3.55846E 00	5.36891E-03	1.84497E 00	0.	2.39264E 00	1.
7.17749E 00	2.85232E 00	1.12629E-02	1.93839E 00	0.	2.37552E 00	1.
7.24061E 00	3.40970E 00	2.38824E-02	1.71821E 00	0.	2.08882E 00	1.
8.12778E 00	4.81720E 00	5.21628E-02	1.59420E 00	0.	1.66422E 00	1.
9.19137E 00	6.34205E 00	1.24577E-01	1.51637E 00	0.	1.20817E 00	1.
1.02052E 01	7.66170E 00	1.84221E-01	1.50400E 00	0.	8.55279E-01	1.
1.12047E 01	8.82033E 00	2.11271E-01	1.49925E 00	0.	6.73867E-01	1.
1.21555E 01	9.88288E 00	2.36286E-01	1.49679E 00	0.	5.39580E-01	1.
1.29609E 01	1.06565E 01	3.17515E-01	1.55348E 00	0.	4.33473E-01	1.
1.35803E 01	1.10804E 01	4.86691E-01	1.63843E 00	0.	3.74843E-01	1.
1.42077E 01	1.16258E 01	6.56800E-01	1.75973E 00	0.	1.65447E-01	1.
1.48320E 01	1.19535E 01	9.69146E-01	1.87106E 00	0.	3.82619E-02	1.
1.61849E 01	1.25585E 01	1.50231E 00	2.12281E 00	0.	1.28150E-03	1.
1.75040E 01	1.29101E 01	2.16356E 00	2.43031E 00	0.	0.	1.
1.91391E 01	1.31356E 01	2.97596E 00	3.02760E 00	0.	0.	1.
2.08622E 01	1.30529E 01	3.63050E 00	4.17875E 00	0.	0.	1.
2.38069E 01	1.31518E 01	4.65153E 00	6.00358E 00	0.	0.	1.
2.99170E 01	1.43234E 01	6.59931E 00	8.99433E 00	0.	0.	1.
3.38842E 01	1.45839E 01	9.07487E 00	1.02254E 01	0.	0.	1.
4.02618E 01	1.37136E 01	8.75791E 00	1.77902E 01	0.	0.	1.
5.22962E 01	1.44124E 01	1.58132E 01	2.20706E 01	0.	0.	1.
7.78804E 01	1.65426E 01	1.55653E 01	4.57725E 01	0.	0.	1.
1.22029E 02	1.79360E 01	5.79645E 01	4.61285E 01	0.	0.	1.
4.04577E 01	9.52972E 00	1.59325E 01	1.49955E 01	0.	0.	1.
1.40038E 02	1.09325E 01	5.10735E 01	7.80323E 01	0.	0.	1.
2.99124E 01	1.04200E 01	3.64314E 00	1.58493E 01	0.	0.	1.
1.25612E 03	1.33602E 01	4.93335E 02	7.49430E 02	0.	0.	0.

INFINITELY DILUTE COARSE GROUP AVERAGE CROSS SECTIONS

XI	MU	N-2N	N-3N	NU	ELAS.REMOVAL	CHI
9.13072E-04	9.12995E-01	8.02885E-02	0.	3.97749E 00	1.21137E-02	3.29078E-0
1.00774E-03	8.91001E-01	2.91763E-04	0.	3.53442E 00	1.13895E-02	1.22546E-0
1.41024E-03	8.38331E-01	0.	0.	3.26847E 00	1.08226E-02	2.11359E-0
2.24386E-03	7.36374E-01	0.	0.	3.11127E 00	1.28004E-02	2.22778E-0
3.30522E-03	6.09072E-01	0.	0.	3.01755E 00	2.25396E-02	1.72339E-0
4.28061E-03	4.93058E-01	0.	0.	2.96381E 00	4.12411E-02	1.10064E-0
5.31713E-03	3.70074E-01	0.	0.	2.93096E 00	6.74430E-02	6.24819E-0
6.24197E-03	2.60413E-01	0.	0.	2.91089E 00	9.56482E-02	3.30061E-0
6.80597E-03	1.93538E-01	0.	0.	2.89674E 00	1.20962E-01	1.66870E-0
7.23833E-03	1.42282E-01	0.	0.	2.89136E 00	1.43071E-01	8.21433E-0
7.66871E-03	9.12757E-02	0.	0.	2.88688E 00	1.63443E-01	3.97855E-0
8.01666E-03	5.00399E-02	0.	0.	2.88417E 00	1.77655E-01	1.90810E-0
8.28482E-03	1.62602E-02	0.	0.	2.88224E 00	1.92635E-01	9.09667E-0
8.40362E-03	4.18206E-03	0.	0.	2.88136E 00	2.00905E-01	4.32105E-0
8.41517E-03	2.81300E-03	0.	0.	2.88083E 00	2.11365E-01	2.04806E-0
8.41517E-03	2.81300E-03	0.	0.	2.88050E 00	2.17281E-01	9.69425E-0
8.41517E-03	2.81300E-03	0.	0.	2.88031E 00	2.21076E-01	4.58496E-0
8.41517E-03	2.81300E-03	0.	0.	2.88019E 00	2.19685E-01	2.16742E-0
8.41517E-03	2.81300E-03	0.	0.	2.88011E 00	2.21348E-01	1.02429E-0
8.41517E-03	2.81300E-03	0.	0.	2.88007E 00	2.41067E-01	4.83973E-0
8.41517E-03	2.81300E-03	0.	0.	2.88004E 00	2.45452E-01	2.28651E-0
8.41517E-03	2.81300E-03	0.	0.	2.88003E 00	2.30805E-01	1.08018E-0
8.41517E-03	2.81300E-03	0.	0.	2.88002E 00	2.42565E-01	5.10274E-0
8.41517E-03	2.81300E-03	0.	0.	2.88001E 00	2.78417E-01	2.41046E-0
8.41517E-03	2.81300E-03	0.	0.	2.88001E 00	3.01870E-01	1.13864E-0
8.41517E-03	2.81300E-03	0.	0.	2.88000E 00	1.60386E-01	5.37865E-0
8.41517E-03	2.81300E-03	0.	0.	2.88000E 00	6.13326E-02	4.30689E-0
8.41517E-03	2.81300E-03	0.	0.	2.88000E 00	5.84573E-02	4.53946E-0
8.41517E-03	2.81300E-03	0.	0.	2.88000E 00	0.	4.78457E-1

F-FACTORS FOR TOTAL CROSS SECTION ADJUSTMENT

INF DILUTE	TEMP	SIG=O 10,0	100,0	1000,0	10000,0
1,35803E 01	300,	9,99557E-01	9,99869E-01	9,99976E-01	1,00000E 00
1,42077E 01	300,	9,81535E-01	9,94445E-01	9,99276E-01	9,99981E-01
1,48320E 01	300,	9,65237E-01	9,87804E-01	9,98415E-01	9,99544E-01
1,61849E 01	300,	9,34119E-01	9,73121E-01	9,96276E-01	9,99360E-01
1,75040E 01	300,	8,84470E-01	9,45558E-01	9,92097E-01	9,99063E-01
1,91391E 01	300,	8,28672E-01	9,09260E-01	9,86234E-01	9,98571E-01
2,08622E 01	300,	7,73212E-01	8,67125E-01	9,77708E-01	9,97482E-01
2,38069E 01	300,	6,92465E-01	7,99898E-01	9,60365E-01	9,95490E-01
2,99170E 01	300,	5,71139E-01	6,89894E-01	9,16740E-01	9,89433E-01
3,38842E 01	300,	5,33840E-01	6,41175E-01	8,90782E-01	9,85587E-01
4,02618E 01	300,	4,66611E-01	6,19626E-01	8,81980E-01	9,84635E-01
5,22962E 01	300,	3,44709E-01	4,92640E-01	7,94998E-01	9,67846E-01
7,78804E 01	300,	2,83630E-01	3,88924E-01	6,27114E-01	9,11291E-01
1,22029E 02	300,	1,25526E-01	2,33701E-01	5,66023E-01	9,05744E-01
4,04577E 01	300,	3,19306E-01	4,38295E-01	7,34877E-01	9,56290E-01
1,40038E 02	300,	1,57961E-01	2,28257E-01	5,02489E-01	8,83820E-01
2,99124E 01	300,	8,68118E-01	9,52266E-01	9,93487E-01	9,99324E-01
1,25612E 03	300,	7,24999E-02	9,14675E-02	2,12456E-01	6,74286E-01

F-FACTORS FOR SCAT CROSS SECTION ADJUSTMENT

GROUP	INF DILUTE	TEMP	SIG=0 10,0	100,0	1000,0	10000,0
12	1,10804E 01	300,	9,99823E-01	9,99947E-01	1,00000E 00	1,00000E 00
13	1,16258E 01	300,	9,92989E-01	9,97917E-01	9,99983E-01	1,00000E 00
14	1,19535E 01	300,	9,86707E-01	9,95619E-01	9,99443E-01	1,00000E 00
15	1,25585E 01	300,	9,73018E-01	9,89989E-01	9,98666E-01	9,99532E-01
16	1,29101E 01	300,	9,53457E-01	9,80012E-01	9,96978E-01	9,99232E-01
17	1,31356E 01	300,	9,32571E-01	9,67526E-01	9,95185E-01	9,99523E-01
18	1,30529E 01	300,	9,19202E-01	9,56615E-01	9,93472E-01	9,99236E-01
19	1,31518E 01	300,	8,94795E-01	9,35808E-01	9,88461E-01	9,98646E-01
20	1,43234E 01	300,	8,25814E-01	8,77998E-01	9,70286E-01	9,96353E-01
21	1,45839E 01	300,	8,19420E-01	8,64398E-01	9,63175E-01	9,95299E-01
22	1,37136E 01	300,	8,29212E-01	8,86378E-01	9,68625E-01	9,96071E-01
23	1,44124E 01	300,	7,52428E-01	8,12925E-01	9,29338E-01	9,89450E-01
24	1,65426E 01	300,	6,93042E-01	7,39475E-01	8,60558E-01	9,72488E-01
25	1,79360E 01	300,	4,56545E-01	5,51675E-01	7,70813E-01	9,56027E-01
26	9,52972E 00	300,	9,37206E-01	9,59186E-01	9,85548E-01	9,97912E-01
27	1,09325E 01	300,	8,34856E-01	8,62169E-01	9,30229E-01	9,86493E-01
28	1,04200E 01	300,	9,87748E-01	9,96031E-01	9,99482E-01	9,99946E-01
29	1,33602E 01	300,	9,09179E-01	9,23891E-01	9,61543E-01	9,92139E-01

F-FACTORS FOR CAP CROSS SECTION ADJUSTMENT

GROUP	INF DILUTE	TEMP	SIG=0 10,0	100,0	1000,0	10000,0
12	4,86691E-01	300,	9,99159E-01	9,99772E-01	9,99953E-01	9,99979E-01
13	6,56800E-01	300,	9,68646E-01	9,90907E-01	9,97997E-01	9,99017E-01
14	9,69146E-01	300,	9,46934E-01	9,83988E-01	9,97327E-01	9,99537E-01
15	1,50231E 00	300,	9,08054E-01	9,67806E-01	9,94552E-01	9,98327E-01
16	2,16358E 00	300,	8,38595E-01	9,36273E-01	9,90745E-01	9,98588E-01
17	2,97596E 00	300,	7,65462E-01	8,95352E-01	9,84628E-01	9,97754E-01
18	3,63050E 00	300,	7,01136E-01	8,51400E-01	9,77615E-01	9,97716E-01
19	4,65153E 00	300,	6,11506E-01	7,80310E-01	9,62373E-01	9,95614E-01
20	6,39931E 00	300,	5,04282E-01	6,81504E-01	9,31791E-01	9,91638E-01
21	9,07487E 00	300,	3,71495E-01	5,83295E-01	8,96714E-01	9,86645E-01
22	8,75791E 00	300,	3,27268E-01	5,78054E-01	8,94327E-01	9,87140E-01
23	1,58132E 01	300,	2,51556E-01	4,70011E-01	8,24248E-01	9,75271E-01
24	1,55653E 01	300,	1,78236E-01	3,28002E-01	6,78691E-01	9,39427E-01
25	5,79645E 01	300,	1,26046E-01	2,62291E-01	6,27474E-01	9,30007E-01
26	1,59325E 01	300,	2,17551E-01	4,30064E-01	7,97604E-01	9,71063E-01
27	5,10735E 01	300,	1,42103E-01	2,68119E-01	6,23949E-01	9,27844E-01
28	3,64314E 00	300,	8,30553E-01	9,41131E-01	9,92104E-01	9,99182E-01
29	4,93335E 02	300,	1,13929E-01	1,62239E-01	3,92918E-01	8,12525E-01

F-FACTORS FOR FISS CROSS SECTION ADJUSTMENT

GROUP	INF DILUTE	TEMP	SIG=0 10.0	100.0	1000.0	10000.0
12	1.63843E 00	300.	9.99385E-01	9.99841E-01	9.99980E-01	1.00000E 00
13	1.75973E 00	300.	9.75624E-01	9.93467E-01	9.99067E-01	9.99985E-01
14	1.87108E 00	300.	9.58350E-01	9.87658E-01	9.98216E-01	9.99662E-01
15	2.12281E 00	300.	9.30483E-01	9.76920E-01	9.96653E-01	9.99369E-01
16	2.43031E 00	300.	8.84147E-01	9.56028E-01	9.93230E-01	9.98419E-01
17	3.02760E 00	300.	8.39331E-01	9.33686E-01	9.90932E-01	9.99249E-01
18	4.17875E 00	300.	7.77187E-01	8.94187E-01	9.83503E-01	9.97381E-01
19	6.00358E 00	300.	7.00485E-01	8.38968E-01	9.73468E-01	9.97028E-01
20	8.99433E 00	300.	6.07161E-01	7.56411E-01	9.49590E-01	9.93976E-01
21	1.02254E 01	300.	5.86811E-01	7.53709E-01	9.48129E-01	9.94001E-01
22	1.77902E 01	300.	5.08301E-01	7.11480E-01	9.31157E-01	9.91792E-01
23	2.20706E 01	300.	4.09948E-01	6.26940E-01	8.92283E-01	9.85692E-01
24	4.57725E 01	300.	3.24111E-01	4.72100E-01	7.43300E-01	9.50971E-01
25	4.61285E 01	300.	2.35569E-01	4.78903E-01	8.30488E-01	9.74676E-01
26	1.49955E 01	300.	2.60290E-01	4.54716E-01	8.02753E-01	9.71697E-01
27	7.80323E 01	300.	2.03685E-01	3.39503E-01	6.75863E-01	9.39644E-01
28	1.58493E 01	300.	9.09247E-01	9.69629E-01	9.95984E-01	9.99585E-01
29	7.49430E 02	300.	1.45130E-01	1.95482E-01	4.23099E-01	8.22907E-01

F-NOUGHT F-FACTORS FOR TOTAL CROSS-SECTION TO BE USED WITH SIG-T FOR ITERATION ON SIG-0

SIG-TOTAL	TEMP	SIG-0 10,0	100,0	1000,0	10000,0
1,35803E 01	300,	9,99751E-01	9,99929E-01	9,99996E-01	9,99999E-01
1,42077E 01	300,	9,89794E-01	9,97066E-01	9,99778E-01	9,99953E-01
1,48320E 01	300,	9,80565E-01	9,93866E-01	9,99152E-01	9,99927E-01
1,61849E 01	300,	9,61411E-01	9,86217E-01	9,98020E-01	9,99399E-01
1,75040E 01	300,	9,29636E-01	9,71276E-01	9,95687E-01	9,99040E-01
1,91391E 01	300,	8,91837E-01	9,50950E-01	9,92871E-01	9,99205E-01
2,08622E 01	300,	8,52808E-01	9,25801E-01	9,88716E-01	9,98600E-01
2,38069E 01	300,	7,90444E-01	8,81005E-01	9,79583E-01	9,97646E-01
2,99170E 01	300,	6,89152E-01	7,98100E-01	9,55572E-01	9,94598E-01
3,38842E 01	300,	6,29261E-01	7,55710E-01	9,40835E-01	9,92589E-01
4,02618E 01	300,	5,78228E-01	7,42029E-01	9,35908E-01	9,92238E-01
5,22962E 01	300,	4,56438E-01	6,30744E-01	8,81923E-01	9,83577E-01
7,78804E 01	300,	3,73321E-01	5,00093E-01	7,55294E-01	9,53234E-01
1,22029E 02	300,	2,16025E-01	3,86707E-01	7,25284E-01	9,50717E-01
4,04577E 01	300,	4,02905E-01	5,63834E-01	8,43782E-01	9,77622E-01
1,40038E 02	300,	2,30500E-01	3,54273E-01	6,76787E-01	9,38998E-01
2,99124E 01	300,	9,27008E-01	9,75353E-01	9,96730E-01	9,99662E-01
1,25612E 03	300,	1,41002E-01	1,90173E-01	4,16972E-01	8,20630E-01

INELASTIC SCATTERING MATRIX

GROUP	DOWN-SCATTERING GROUP I+J					
	0 7 14	1 8	2 9	3 10	4 11	5 12	6 13
	5.39999E-01 5.17319E-02 7.31486E-05	3.45679E-02 2.27267E-02 4.28691E-05	6.56048E-02 9.31400E-03	1.74312E-01 3.65880E-03	2.22735E-01 1.40071E-03	1.77546E-01 5.27906E-04	1.05109E-01 1.97076E-04
	6.74834E-01 5.66245E-02 7.17020E-05	8.07435E-02 2.37921E-02 4.19486E-05	2.26880E-01 9.48930E-03	3.77850E-01 3.66635E-03	3.57681E-01 1.38965E-03	2.35277E-01 5.20552E-04	1.23741E-01 1.93613E-04
	8.94134E-01 3.16272E-02 3.66365E-05	2.56086E-01 1.28193E-02 2.14045E-05	3.23907E-01 5.00202E-03	3.67702E-01 1.90712E-03	2.71716E-01 7.16980E-04	1.53390E-01 2.67258E-04	7.33044E-02 9.91069E-05
	1.19265E 00 1.15420E-02 1.23720E-05	4.45702E-01 4.53367E-03 7.22019E-06	2.75585E-01 1.73555E-03	2.20045E-01 6.54079E-04	1.30297E-01 2.44174E-04	6.41229E-02 9.06287E-05	2.81664E-02 3.35207E-05
	1.15445E 00 2.58258E-03 2.44089E-06	4.92936E-01 9.60996E-04 1.42366E-06	2.69117E-01 3.49073E-04	8.83898E-02 1.37021E-04	5.23618E-02 4.84638E-05	2.07223E-02 1.79334E-05	6.74015E-03 6.62077E-06
	9.49036E-01 1.20652E-03 0.	3.73068E-01 4.48441E-04 0.	2.12912E-01 4.63513E-05	7.74973E-02 3.53868E-05	3.30108E-02 0.	1.18320E-02 0.	5.12700E-03 0.
	8.46115E-01 5.26240E-04 0.	2.36535E-01 2.93471E-04 0.	5.84506E-02 5.31047E-06	3.51967E-02 1.07232E-06	1.78012E-02 0.	8.93762E-03 0.	4.30888E-03 0.
	6.01810E-01 5.89151E-04 0.	2.48062E-01 1.92169E-04 0.	3.19558E-03 0.	3.06314E-04 0.	1.04107E-04 4.39670E-08	2.28034E-05 0.	9.96284E-04 0.

INELASTIC SCATTERING MATRIX

SOURCE GROUP I	DOWN-SCATTERING GROUP I+J 0 / 7 / 14	1 / 8	2 / 9	3 / 10	4 / 11	5 / 12	6 / 13
9	4.10434E-01 0. 0.	2.07272E-01 5.25837E-07 0.	5.31749E-02 0.	2.97389E-03 0.	4.17254E-06 0.	5.42831E-06 0.	2.89762E-06 0.
10	3.34085E-01 5.87701E-05 0.	1.39038E-01 2.85677E-05 0.	3.84830E-02 0.	2.06645E-02 0.	6.58065E-03 0.	5.49384E-04 0.	9.21847E-05 0.
11	2.75189E-01 9.46396E-05 0.	1.53763E-01 0. 0.	0. 1.70746E-05	9.68438E-04 0.	2.14296E-03 0.	1.12467E-03 0.	1.73508E-04 0.
12	1.74638E-01 0. 0.	2.00205E-01 0. 0.	0. 0.	0. 0.	0. 0.	0. 0.	0. 0.
13	3.67296E-02 0. 0.	1.04100E-01 0. 0.	2.46175E-02 0.	0. 0.	0. 0.	0. 0.	0. 0.
14	0. 0. 0.	1.30085E-02 0. 0.	1.57871E-02 0.	6.12192E-03 0.	2.89234E-03 0.	4.52034E-04 0.	0. 0.
15	0. 0. 0.	0. 0.	0. 0.	0. 0.	7.50749E-04 0.	5.19263E-04 0.	1.14835E-05 0.

)ENDR CASE ID NO, PU239 CASE SEQUENCE NO, 1 050771 0326,1 PAGE NO, 61

N-2N MATRIX

SOURCE GROUP I	DOWN-SCATTERING GROUP I+J 0	1	2	3	4	5	6
	7	8	9	10	11	12	13
	14						
1	4.19518E-05	1.69762E-03	1.30846E-02	3.37581E-02	4.23464E-02	3.33760E-02	1.96245E-02
	9.61887E-03	4.21522E-03	1.72491E-03	6.76974E-04	2.59025E-04	9.75898E-05	3.64246E-05
	1.35180E-05	7.92155E-06					
2	2.54031E-06	3.04401E-05	1.03186E-04	1.53437E-04	1.34335E-04	8.42434E-05	4.29474E-05
	1.92764E-05	8.00361E-06	3.16904E-06	1.21906E-06	4.60786E-07	1.72324E-07	6.40302E-08
	2.36983E-08	1.38581E-08					

CASE SEQUENCE NO. 1 050771 0326,1

ELASTIC SCATTERING MATRIX

DOWN-SCATTERING GROUP I+J

)ENDR CASE ID NO. PU239

SOURCE GROUP

)ENDR CASE ID NO. PU239 CASE SEQUENCE NO. 1 050771 0326,1 PAGE NO. 63

A GMUG FILE HAS BEEN CREATED FOR MATERIAL NUMBER 1104

CLASS NO. 1 HAS 1 BLOCKS. CLASS WORD = 000250100001 CLASS ID IS I10401

CLASS NO. 2 HAS 2 BLOCKS. CLASS WORD = 000270100002 CLASS ID IS I10402

CLASS NO. 3 HAS 1 BLOCKS. CLASS WORD = 000320100001 CLASS ID IS I10403

CLASS NO. 4 HAS 1 BLOCKS. CLASS WORD = 000340100001 CLASS ID IS I10404

CLASS NO. 29 HAS 1 BLOCKS. CLASS WORD = 000360100001 CLASS ID IS I10405

CLASS NO. 6 HAS 1 BLOCKS. CLASS WORD = 000400100001 CLASS ID IS I10406

CLASS NO. 7 HAS 1 BLOCKS. CLASS WORD = 000420100001 CLASS ID IS I10407

RECORD OF PROCESSOR TIME

Y	PROCESSOR TIME
	SECONDS
RUN SUBROUTINES	22,61
NITIAL CALCULATIONS	15,74
1,2 UNRESOLVED RESONANCE CALCULATIONS	11,15
SMOOTH DATA AVERAGING	24,14
SONANCE ULTRA-FINE CALCULATION AND AVERAGE	463,44
N-2N, ELASTIC MATRIX GENERATION	30,49
TANDARD OR FCC	3,37
P CROSSSECTION PLOTTING	0,00
SSOR TIME	570,94

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APPENDIX A

USER ERROR INDEX

Error No.	Called In SUB.	Meaning
4	SKIPMT	Read an MT value different from the reaction type being skipped - i.e., cards out of order or programming error
4	SKIPMF	Same except file number MF is wrong
4	SKPMAT	Same except material number MAT is wrong
5	RESTOR	Overlay Error, MF or MAT = 0 or MT not in order
99	RREC	NT not defined
100	RREC	JT out of range 1-6 (record type)
101	RREC	Mode out of range 1-3
102	RREC	Temp. not in range given in data
103	RREC	Interpolation table too long or 0
104	RREC	List too long or 0
105	RREC	Tabulation too long or less than 2
106	RREC	Improper temp. dependence
107	RREC	MAT, MF, MT incorrect
130	TERP2	Energies are not in increasing order (table of x)
131	TERP2	Energies are not in increasing order (values of interpolated points xp)
132	TERP2	Calls for interp. at breakpoint k larger than the number of points given Ni. i.e. NBT(Ni) is too small

Error No.	Called in SUB.	Meaning
133	TERP1	Interpolation code out of range
134	TERP1	Zero or negative value can't be interpolated by log.
135	TERP1	X1 = X2, discontinuity
300	URESXS	Atomic weight, AWR, is zero. Would result in infinite loop if not aborted.
400	SUB1	$I_{wit} < 0$ specified material, MAT, not on NPOST tape
500	FNDMAT	Material is not on tape mounted or more than 10 cards in a row have MAT = 0. Wrong tape mounted.
500	SMXSAV	Reaction types (MT) not listed in increasing order. (Exception - inelastic values)
1011	READ3	File number (MF) of first card = 0
1102	SUB1	Asked for resonance calculation but no resonance data is given in File 2.
1111	ELASM	Asked for elastic matrix and σ_{er} but not elastic infinite dilue (MT=2).
1112	ELASM	Asked for elastic matrix for hydrogen - not possible now.
1153	N2NMAT	N-2N File 5 data given in form other than LF=1, 3 or 9. Can't handle. Check File 5 of material.
1250	MUXI	Asked for μ and ξ calculation but not elastic scattering (MT=2).
1251	MUXI	Asked for μ calculation but μ values were not specified in ICT=8.

Error No.	Called in SUB.	Meaning
1252	MUXI	Asked for ξ calculation by direct averaging but ξ values were not specified in ICT=7.
1600	NUBAR	Asked for ν calculation but not infinite dilute fission (MT=18).
1601	INELSM	Asked for inelastic matrix but not the total inelastic cross section.
1602	N2NMAT	Asked for N-2N matrix but not the total N-2N cross section.
1603	N2NMAT	Asked for N-2N matrix but no data is given in file 5
1701	INITL	$\sigma_o < 0.0$ - can't take log
1702	NRESXS	Input $\sigma_o = 0$, converted to 0.1

APPENDIX B

CHECKOUT STATUS

There are 10 general areas in the ENDRUN code in which a programming or input error might occur: General, Data Source, Flux, Smooth, Unresolved, Resolved, Overlap, Non-cross section, Matrices, and Output. An attempt has been made to check out each of these areas as thoroughly as possible. For the benefit of new users, the list of options below shows those which have been run successfully to date (checked) and those which so far have not been explicitly checked. While some of the "options" listed are actually tests of the maximum limits or combinations of several options, it should be noted that not all of the maximum limits or all of the options have been run in the same case. The authors would appreciate notification of any anomalies that appear in option combinations not previously tested.

1. General
   - ✓ - 100 coarse groups
   - ✓ - 30 fine groups/coarse group
   - ✓ - starting lethargy other than 0.0
   - - use of ENDF/B rather than sum total for self-shielding
   - - use of ENDF/B total as output, adjusting σ_s for consistency

2. Data Source
   - ✓ - ENDF/B data on punched cards
   - - BCD tape for a single material
   - - binary tape created by DAMMET containing several materials
   - ✓ - NPOST compressed binary tape

3. Flux
   - - entirely 1/E flux spectrum (FSCL > energy at SLETH)
   - ✓ - 1/E spectrum combined with a fission spectrum at high energies
   - ✓ - input flux spectrum from punched cards
   - ✓ - intermediate output of fine group energies and fluxes

4. Smooth

- a single reaction only (without total cross section)
- a single reaction, also included as total
- ✓ - all smooth cross section contributions
- ✓ - 2 ENDF/B reaction MT values included in the same ICT
- ✓ - self-shielded smooth contribution

5. Unresolved

- ✓ - infinitely dilute calculation only
- self-shielding (RAPTURE) with 4 σ_os, 3 T's,
- ✓ - 30 energy points
- other (non-RAPTURE) unresolved calculation options
- ✓ - punched card output of point-wise unresolved contribution
- rerun from previously punched cards
- maximum of 15 ℓ,j states (applies to entire material)
- ✓ - maximum of 6 isotopes
- ✓ - several energy ranges
- ✓ - overlap correction below energy ELAPC
- ✓ - intermediate output of coarse and fine group unresolved averages

6. Resolved

- ✓ - 1 resonance, infinitely dilute only
- ✓ - many resonances, infinitely dilute
- ✓ - self-shielding with 5 σ_os, 3 T's
- ✓ - maximum of 7 resolved resonance energy ranges
- ✓ - maximum of 6 isotopes
- ✓ - intermediate output of coarse and fine group resolved resonance averages

7. Overlap

√ - resolved and unresolved resonance ranges ending in the same coarse group, but no energy overlap

- actual energy overlap between resolved and unresolved but ending in the same coarse group

- energy overlap extending more than one coarse group

√ - overlap of resolved resonance contribution with smooth

√ - overlap of unresolved resonance contribution with smooth

8. Non-cross section

√ - Averaging of μ and ξ directly from ENDF/B data

√ - LDXI=1, average of ξ based on theoretical value and anisotropic correction

√ - calculation of ν from polynomial representation

- calculation of ν by interpolation

√ - secondary fission spectrum based on given ENDF/B θ temperature (Fission, Maxwellian, or Watt spectra)

√ - secondary fission spectrum when θ is energy-dependent (LECHI≠0)

√ - secondary fission spectrum when more than one type of spectrum is used (NK>1)

9. Matrices

√ - calculation of σ_d

√ - lethargy gain indicator

√ - elastic matrix

√ - inelastic matrix LF=3 level data

LF=9 energy-dependent Maxwellian

- n,2n matrix LF=1 arbitrary tabulated function

LF=9

LF=10 Watt spectrum

√ - combined n,2n and n,3n matrices

√ - all matrices combined into inelastic matrix

√ - maximum matrix size of 70x50 (49 downscatter groups)

10. Output

✓ - standard printout

✓ - GMUG compressed binary file tape

- plotting of cross sections

- plotting of f-factors

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