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TDOWN - A CODE TO GENERATE COMPOSITION AND SPATIALLY DEPENDENT CROSS SECTIONS

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ABSTRACT

1. Name: TDOWN
2. Computer: GE 635
3. Problem Solved: TDOWN generates spatial and composition dependent cross section sets from a Bondarenko type, generalized cross section file called GMUG. A TDOWN problem can be a simple description of material compositions with an input flux spectra or a problem can consist of a multi-regional two-dimensional reactor description with several 0- or 1-dimensional flux solutions to provide the flux for spectral adjustments of the cross section sets.
4. Method of Solution: TDOWN uses the rapid cross section adjustment procedure and a generalized file. For each material, the file contains the groupwise values of: infinitely-dilute cross sections; resonance self-shielding factors which are tabulated for temperatures and a range of σ_0 's - the material composition dependent parameter; and scattering matrices.

Self-shielding of a cross section is accomplished by computing σ_0 and using interpolation routines to determine the self-shielding factor for the σ_0 and input temperature. Self-shielding is an iterative procedure with the convergence criteria specified in the input. Spectral adjustments to the elastic removal are carried out directly if the flux sets are input. 0 or 1-dimensional flux solutions may be specified to generate the flux sets. The flux solutions are iterated until spectral adjustments converge to the input criteria.
5. Restrictions on the Complexity of the Problem: Most of the restrictions on TDOWN are due to the limitations of the linked codes. Some of these limitations include: a generalized file has a maximum of 100 energy groups, and up to 120 material cross section sets may be output.
6. Typical Running Time: Problems with all the flux spectra input use a maximum of a few minutes on the GE635. A 29 energy group problem generating 100 materials in 15 compositions with the flux spectra computed by two 1-dimensional flux solutions, 9 iterations each, required .3 hours of computer processor time.

7. Unusual Features of the Program: TDOWN gives the user flexibility in determining the detail a particular output cross section file will have with respect to composition and spatial effects. Output cross sections sets from the compositions are not automatic; each set is selected from particular compositions and then the user can apply any spectral set to correct the elastic removal. If the problem requires flux solutions and consequently regional descriptions, compositions may be defined outside of the regions.
8. Related or Auxiliary Programs: Data for the generalized file - GMUG is generated by the ENDRUN code.
9. Status: TDOWN is in production status and is executed from tape.
10. References: 1) C. L. Cowan, B. A. Hutchins, and J. E. Turner, "TDOWN - A Code to Generate Composition and Spatially Dependent Cross Section", GEAP-13740, August, 1971.
2) Group Constants for Nuclear Reactor Calculations, edited by I. I. Bondarenko, Consultants Bureau, New York, 1964.
3) B. A. Hutchins, C. L. Cowan, M. D. Kelley, and J. E. Turner, "ENDRUN-II, A Computer Code to Generate a Generalized Multigroup Data File from ENDF/B", GEAP-13704, March 1971.
11. Machine Requirements: The program requires 32K of computer memory on the GE635. This includes a 10K overlap with the loading routines. In addition to the card reader and printer devices, three tape handlers and six files on a peripheral device (discs at GE) are required.
12. Programming Languages Used: TDOWN is written in FORTRAN.
13. Operating System: GECOS III with the FORTRAN compiler.
14. Other Programming or Operating Information: Primary changes to convert this program to another machine would be the input/output routines and peripheral assignments.

SECTION I

INTRODUCTION

The General Electric rapid cross section adjustment procedure was developed to use the Bondarenko⁽¹⁾ approach in formulating multigroup cross sections. Spatial and composition dependent cross sections for a particular reactor design are prepared from a generalized cross section file by the use of resonance self-shielding factors (through interpolation routines) and adjustment of the elastic scattering cross section for the local neutron flux spectra. This method avoids expensive and repetitive direct averaging of the basic nuclear data for every reactor design, while providing sufficient accuracy for most design calculations.

TDOWN was specified to give the user maximum flexibility in using the rapid cross section adjusting approach. Problem descriptions can vary from a single composition with fluxes input, to a two-dimensional, multiregional problem requiring several one-dimensional flux solutions and resulting in a set of microscopic cross sections for each material in each region.

Among some of the code capabilities are the following:

- 1) Sets of neutron flux spectra may be input, calculated by zero or one-dimensional diffusion solutions, or a combination of input and calculations.
- 2) Flux spectra corrections to the elastic removal cross section for any material can be carried out using any flux set.
- 3) Materials in similar compositions with a similar neutron flux spectra need only have one representative set of effective, microscopic cross sections, and, at the discretion of the code user, the representative sets are selected for output.

With the aforementioned capabilities and other input options, the code user can easily specify the detail, with respect to composition and spatial effects, of the cross section sets generated by TDOWN.

The generalized (GMUG) file used by TDOWN will ordinarily be prepared from the ENDF/B libraries⁽²⁾ by the ENDRUN code.⁽³⁾ For each material, this file will normally contain the following information:

- a) Multigroup infinitely-dilute microscopic cross sections, scattering data and reaction parameters,
- b) Self-shielding factors for specific groups as functions of material temperature and the generalized composition dependent parameters, σ_0 , and
- c) Transfer matrices for inelastic scattering, elastic scattering and (n,2n) reactions.

SECTION II

GENERAL DESCRIPTION OF TDOWN APPLICATION AND THEORY

The TDOWN code is used to generate multigroup cross sections for a specific set of material compositions and neutron flux spectra corresponding to a 0, 1, 2, or 3 dimensional neutronics problem. Utilization of TDOWN presupposes the existence of a generalized multigroup cross section file, called a GMUG file.* Therefore, the TDOWN input is directly linked to the output from the ENDRUN code.⁽³⁾ The principal modifications to the GMUG data performed by TDOWN are the following:

- 1) Self-shielding factors (f-factors) are used to modify the infinitely dilute cross sections for fission, capture, elastic scattering and total reactions. The f-factors are dependent upon the temperature of the material and the composition in which the material is found.
- 2) The elastic removal cross section is corrected for the energy distribution of the neutron flux seen by the material. The neutron flux spectra may be input or determined by a fundamental mode or one-dimensional diffusion theory calculation.

The computations described above may be carried out over a broad range of detail, at the option of the user. The total number of cross section sets included in the output file may be large if the problem contains many compositions, zones and materials and if effective cross sections are obtained for each material in each composition and zone.

*A description of a GMUG file is given in Part 1 of Appendix A.

This number becomes unmanageable for 2- and 3-dimensional neutronics problems. However, TDOWN is designed to allow the user to take advantage of the fact that it is not generally necessary to apply the self-shielding and spectral modifications to every material in every composition and zone. For example, in a reactor containing several core enrichment zones and blankets a single self-shielding correction may be sufficient for iron in all core zones and the blankets. However, the spectral modification to elastic removal would be applied separately to iron in the core and in the blankets.

This broad range of detail optionally available in TDOWN is achieved by specifying particular sets of compositions and flux spectra which are used for the modifications, and each modification is applied independently of the other. Thus a material to be put on the output file is specified by a) the GMUG material used for the source of the cross sections, b) the composition set and material temperature applied for self-shielding, c) the spectral set applied for elastic removal, and d) heterogeneity effect information. A two-dimensional reactor description is input but is only for the aid of the user and for performing one-dimensional flux solutions. Composition sets may, or may not, correspond to compositions in the two-dimensional description. This permits a single TDOWN problem to provide output data sets for the same material in the same composition at different temperatures, or even cross section sets for different neutronics problems. The flux spectra sets may be obtained from zero- or one-dimensional solutions internal to TDOWN or from input. The one-dimensional solutions are performed through specified rows of zones in the two-dimensional description. An example of a TDOWN problem is given in Section 3.5.

Figure 1 shows a generalized flow diagram of the TDOWN procedures and computations. The first step in the execution of a TDOWN problem is processing the input and reading the GMUG file. In this step all compositions, regions, geometry, and flux solution are defined from the input specifications. Data on the GMUG file is read and stored for each material used in the problem.

FIGURE 1

GENERALIZED FLOW DIAGRAM OF TDOWN COMPUTATIONS AND PROCEDURES*

*A dashed line means an iterative step

Self-shielded cross sections for the total, transport, scattering, capture and fission reactions are computed for those groups for which correction factors (f-factors) are given in the GMUG file. Otherwise, the infinitely-dilute reaction values on the GMUG file are used directly as the group averaged cross sections.

The self-shielding computations for a given composition set start with the determination of the self-shielding parameter for the i -th group and m -th material, $(\sigma_o)_{i,m}$, (i.e., the sum of the total cross sections of all materials, other than material m , divided by the atom concentration of material m):

$$(\sigma_o)_{i,m} = \frac{1}{N_m} \sum_{n \neq m} (\sigma_t)_{i,n} N_n$$

where $(\sigma_t)_{i,n}$ is the total cross section of the i -th group and n -th material, N_n is the atom concentration of the n -th material and N_m is the atom concentration of the material for which the self-shielded cross sections are being computed. Note: $(\sigma_t)_{i,n}$ may, itself, be self-shielded, requiring an iterative process to converge on $(\sigma_o)_{i,m}$. The iteration number and convergence criteria is specified in the TDOWN input.

Heterogeneity is treated in TDOWN by using an optional procedure for calculating the σ_o 's based upon the Bell rational approximation.⁽⁴⁾ The optional treatment is limited to the cylindrical or slab cell prescriptions described in Section 3.2.1.

Following the determination of $(\sigma_o)_{i,m}$ values, resonance self-shielding correction factors are computed by interpolating between the f-factors which are tabulated for discrete values of the temperature and σ_o . The f-factor interpolation on σ_o is carried out by means of a Taylor series expansion about neighboring values whereas the interpolation on the temperature is based upon a simple logarithmic proportionality between the tabulated values. The f-factors may be specified (in the GMUG file) for up to three temperatures and five values of σ_o . It is again noted that the GMUG infinitely-dilute cross sections are used directly if the correction factors are not provided.

The self-shielding correction factors for total, transport, scattering, capture and fission reactions are used to adjust the appropriate infinitely-dilute cross sections. The scattering correction factor is also used to adjust the elastic removal cross section and transfer terms (if applicable).

The neutron flux spectra sets used in TDOWN to adjust the elastic removal cross sections and for the calculation of the fission neutron spectra may be input or obtained from fundamental mode or one-dimensional diffusion theory calculations. A series of one-dimensional flux solutions may be run to obtain the spectra in various zones of a multi-dimensional reactor system, specified in a two-dimensional geometry. The one-dimensional solutions are performed through a line of regions and are all independent of the others (see Section 3.5). The number of neutron flux solutions may be kept small by the judicious choice of key regional neutron flux sets of importance to the adjustment of the removal cross sections. Cross sections used in the flux solutions have been self-shielded for the composition in the local zone.

The adjustment to the elastic removal cross section is based upon a simple linear relationship between the slowing down density and the lethargy in neighboring groups. This expression for the adjusted removal

$$(\sigma_{er})_{i,m}^{\text{adjusted}} = (\sigma_{er})_{i,m}^o \int_{u_i - V}^{u_i} \frac{1}{\xi_{i,m}} \frac{\psi(u)}{\psi_{i,m}} \left[\frac{e^{-(u_i - u) - \alpha_m}}{1 - \alpha_m} \right] du$$

where $(\sigma_{er})_{i,m}^o$ = the elastic removal cross section for the i-th group and m-th material based upon a 1/E flux representation

$$(\sigma_{er})_{i,m}^o = \frac{\xi_{i,m} \sigma_{s,i,m}}{\Delta u_i}$$

$\frac{\psi(u)}{\psi_{i,m}}$ = Ratio of the slowing down density as a function of lethargy to the slowing down density for the i -th group and m -th material.

$$\begin{aligned}\frac{\psi(u)}{\psi_{i,m}} &= \frac{\xi_m(u) \sigma_{s,m}(u) \phi(u)}{\xi_{i,m}(\sigma_{s,i,m} \phi_i / \Delta u_i)} \\ &= 1 + a_{i,m} + b_{i,m}(u - u_i)\end{aligned}$$

$$\begin{aligned}V &= \ln \frac{1}{\alpha_m} \quad \text{if } \ln \frac{1}{\alpha_m} < \Delta u_i \\ &= \Delta u_i \quad \text{otherwise}\end{aligned}$$

The $a_{i,m}$ and $b_{i,m}$ are constants to be determined and the remaining terms have the usual meanings, with the fluxes corresponding to a given flux set.

Since the flux solutions themselves are affected by this elastic removal modification, provision is made to iterate between the solutions and the modification. The final spectral modifications for output cross sections are made after these iterations are completed (if iterations are asked for).

The principal output from the TDOWN code is an effective, multi-group data file in the MUG format.* This file will generally be for a specific reactor description, although the flexibility of TDOWN makes it also capable of generating a data file for parametric studies. The following chapters describe the TDOWN calculations and options in more detail.

*A description of a MUG file is given in Part 2 of Appendix A.

SECTION III

DETAILED DESCRIPTION OF TDOWN THEORY AND PROCEDURES

3.1 Generalized Input Data File - GMUG

The TDOWN code requires input from a generalized multigroup cross section file, called GMUG, generally consisting of from 20 to 100 groups. An independent, single-material GMUG file is output directly by the ENDRUN code, but invariably the GMUG file used in TDOWN will contain many materials. The PUNT code, a GMUG file maintenance routine described in Appendix C, combines the single-material files into one file. Each material on this file can be considered as an independent cross section library. That is, the materials are not necessarily related by any common composition, spectra or problem limitations other than the specifications of the energy group structure. In addition, the fission neutron spectrum, elastic removal reactions, inelastic matrix length, etc., are peculiar to each material.

The generalized data on the GMUG file includes the following information for each material:

- 1) Identification and control parameters that indicate the presence or absence of arrays (f-factors or scattering matrices), starting and ending groups for arrays, and values of σ_0 and temperature;
- 2) Infinitely dilute group-average cross sections for elastic scattering (σ_s), capture (σ_c), fission (σ_f), total (σ_T), inelastic (σ_{in}), (n,2n), (n,3n) and elastic removal (σ_{er}) reactions;
- 3) Group-average values of the average lethargy loss per collision by elastic scattering ($\bar{\xi}$), the average cosine of the elastic scattering angle ($\bar{\mu}$), the average number of neutrons released per fission ($\bar{\nu}$), and the fraction of fission neutrons emitted in each energy group (χ);

- 4) A lethargy gain indicator (LGI) which identifies the method (that is, the extent of the interpolation on the integrated fluxes) used in the elastic removal adjustment;
- 5) Self-shielding f-factors for each group as functions of σ_0 and temperature for iterating on $\sigma_0(f_t)$;
- 6) Individual self-shielding f-factors by group and as functions of the generalized parameter σ_0 and temperature for transport (f_{Tr}), elastic (f_s), capture (f_c) and fission (f_f) reactions;
- 7) Transfer matrices for elastic scattering, inelastic scattering and (n,2n) reactions.

A listing of a complete GMUG material (containing all the parameters listed above) is given in Appendix A.

Each material which is to be used in the TDOWN problem is read from the GMUG file and stored. No attempt is made initially to combine the elastic, inelastic or (n,2n) matrix terms or to modify any of the other cross sections or reaction parameters except that the matrix terms are compacted for more convenient storage.

The atomic weight of each material is checked prior to the processing of the elastic matrix terms. For $A \leq 1.1$, the material is assumed to be hydrogen and the scattering matrix is determined by a Selengut-Goertzel calculation. The Selengut-Goertzel computations are described in Appendix B.

3.2 Resonance Self-Shielding

Composition and temperature dependent cross sections are computed for each material and for each energy group for which the self-shielded f-factors are provided. Should the f-factors not be included, the infinitely-dilute cross sections from the GMUG file are used directly as the group-averaged cross section values.

Because the compositions in the different reactor regions are often at least slightly dissimilar, it is theoretically possible for one material to be specified by a different set of cross sections for each region. However, it is rare that such distinctions are required and for this reason considerable flexibility has been included in TDOWN to reduce the amount of unnecessary data output. Thus, the same composition can be used in more than one region and a cross section set for a given material can be used in more than one composition. An example of this interchangeability of materials and compositions is given in Section 3.5.

3.2.1 Computation of the Self-Shielding Parameter, σ_o

The f-factors are provided as a function of the temperature and the self-shielding parameter, σ_o . Thus, it is necessary to compute the σ_o values for each group i and material m as appropriate. This computation is carried out in the usual manner, by composition, as follows:

$$(\sigma_o)_{i,m} = 1/N_m \sum_{n \neq m} N_n (\sigma_t)_{i,n} \quad 2.1$$

where $(\sigma_t)_{i,n}$ is the total cross section for the i -th group of the n -th material

N_n is the atom concentration of the n -th material, and

$\sum_{n \neq m}$ is the summation over all the materials within the composition being considered except for material m

It will be shown that $(\sigma_t)_{i,n}$ is a function of $(\sigma_o)_{i,n}$ (if f-factors are provided for $(\sigma_t)_{i,n}$) and thus the computation in Equation 2.1 is an iterative procedure subject to certain input convergence criteria and iteration limitations (see Section 3.2.4).

Heterogeneity will be treated in TDOWN by an optional calculation of the self-shielding parameter, σ_o , based upon the Bell rational approximation.⁽⁴⁾ If the input indicator, δ_H (this indicator will be provided by material), is non zero, an effective value of σ_o will be computed for either a simple plate cell or a simple rod cell according to the cell geometry shown in Figure 2. This computation is given as follows:

PLATE CELL - HETEROGENEITY CORRECTION TO σ_o ($\delta_H=2$)

$$(\sigma_o)_{i,m} = \frac{\Sigma_{i,1}}{N_m} - (\sigma_t)_{i,m} + \frac{1}{N_m(2D_2+1/\Sigma_{i,2})} \quad 2.2$$

CYLINDRICAL CELL - HETEROGENEITY CORRECTION TO σ_o ($\delta_H=1$)

$$(\sigma_o)_{i,m} = \frac{\Sigma_{i,1}}{N_m} - (\sigma_t)_{i,m} + \frac{1}{N_m \left(\frac{D_2^2}{D_1} + 1/\Sigma_{i,2} \right)} \quad 2.3$$

$$\text{where } \Sigma_{i,1} = \sum_n f_n N_n (\sigma_t)_{i,n}$$

$$\Sigma_{i,2} = \sum_n (1-f_n) N_n (\sigma_t)_{i,n}$$

D_2 and D_1 = cell dimension from Figure 2

f_n = fraction of smeared atom concentration
for the n-th material in cell region 1

$$f_{n=m} = 1$$

Figure 2. Cell Models for the Computation of the Self-Shielding Cross Section, σ_0

and $\sum_n$ = summation over all materials within the composition being considered.

The derivation of the heterogeneity corrections is given in Appendix D).

The condition that all of material m (for which the σ_o values are being computed) must be located in region 1 is necessary to the definition of a heterogeneity problem. However, this does not preclude other materials from being in both regions (e.g., oxygen associated with fuel and oxygen associated with a moderator such as beryllium). For these materials, however, the self-shielding parameter will be determined as in Equation 2.1.

3.2.2 Computation of Self-Shielding f-factors for Specific σ_o Values

Self-shielding factors for a particular σ_o are determined by an interpolation calculation between the tabulated f-factor values*. These coefficients are given for at least two and for up to five discrete values of σ_o . If three or more discrete values of σ_o are used the following relationship must hold, for all groups and materials having f-factors

$$\Delta = \ln \left[(\sigma_o)_{\text{Tab}_{i,m}}^{k+1} \right] - \ln \left[(\sigma_o)_{\text{Tab}_{i,m}}^k \right] \quad 2.4$$

for $(K_{\min} \leq k \leq K_{\max} - 1)$

where $(\sigma_o)_{\text{Tab}_{i,m}}^k$ = The k -th discrete tabulated value of σ_o for the i -th energy group and m -th material

$K_{\min}$ = Indicator for the smallest value of σ_o for which f-factors are provided.

*The discussion in Sections 3.2.2 and 3.2.3 is concerned only with those materials and energy groups for which the f-factors are provided. It is again noted that if the f-factors are omitted the interpolation calculation is skipped and the infinitely-dilute cross sections from the GMUG file are used directly as the group averaged cross sections.

$K_{\max}$ = Indicator for the largest value of σ_o
for which f-factors are provided.

Δ = A constant equal to the logarithmic decrement
between the first two discrete tabulated values of σ_o

The conditional relationship for Δ (i.e., that the logarithmic decrement be a constant) is not a serious limitation on the code specifications, but it does require that care be taken in selecting the discrete values of σ_o to be used in preparing the GMUG material.

To determine the f-factor coefficient for a particular σ_o it is necessary to locate the σ_o in the table of discrete values and, if the f-factor coefficient is temperature dependent, it is also necessary to identify the two temperatures, T_1 and T_2 , which bracket the specified material temperature.

The interpolation calculation is based upon a Taylor series expansion of the f-factor coefficients about neighboring values of $(\sigma_o)_{\text{Tab},i,m}^k$. The derivation of this expansion is given in Appendix E. The f-factors, $f(\sigma_o, T_j)$, are determined for five different ranges of values for σ_o . These ranges are listed below where the energy group, material indicators and reaction type (e.g., scattering, fission, etc.,) have been omitted for convenience.

$$1) \quad \underline{\ln(\sigma_o) \leq \ln\left((\sigma_o)_{\text{Tab}}^{K_{\min}}\right)}$$

$$f(\sigma_o, T_j) = f\left((\sigma_o)_{\text{Tab}}^{K_{\min}}, T_j\right) \quad 2.5$$

for $j = 1, 2$ (temperature brackets)

$$2) \quad \underline{\ln(\sigma_o) \geq \ln\left((\sigma_o)_{\text{Tab}}^{K_{\max}}\right) + \Delta}$$

$$f(\sigma_o, T_j) = 1.0 \quad 2.6$$

for $j = 1, 2$ (temperature brackets)

$$3) \quad \ln \left((\sigma_o)_{\text{Tab}}^{K_{\min}} \right) < \ln(\sigma_o) \leq \ln \left((\sigma_o)_{\text{Tab}}^{K_{\min}} \right) + \Delta$$

$$\begin{aligned} f(\sigma_o, T_j) &= f \left((\sigma_o)_{\text{Tab}}^{K_{\min}+1}, T_j \right) \left[1 - \left(\frac{\delta_1}{\Delta} \right)^2 \right] \\ &+ f \left((\sigma_o)_{\text{Tab}}^{K_{\min}}, T_j \right) \left[-\frac{\delta_1}{2\Delta} + \frac{1}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \right] \\ &+ f \left((\sigma_o)_{\text{Tab}}^{K_{\min}+2}, T_j \right) \left[\frac{\delta_1}{2\Delta} + \frac{1}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \right] \end{aligned}$$

2.7

for $j = 1, 2$ (temperature brackets)

$$\text{where } \delta_1 = \ln(\sigma_o) - \left(\ln \left((\sigma_o)_{\text{Tab}}^{K_{\min}} \right) + \Delta \right)$$

$$\text{and } f \left((\sigma_o)_{\text{Tab}}^{K_{\min}+2\Delta}, T_j \right) = 1, \text{ if } \ln(\sigma_o)_{\text{Tab}}^{K_{\min}} + \Delta = \ln(\sigma_o)_{\text{Tab}}^{K_{\max}}$$

$$\text{if } f(\sigma_o, T_j) < f \left((\sigma_o)_{\text{Tab}}^{K_{\min}}, T_j \right) \text{ set } f(\sigma_o, T_j) = f \left((\sigma_o)_{\text{Tab}}^{K_{\max}}, T_j \right)$$

$$4) \quad \ln \left((\sigma_o)_{\text{Tab}}^{K_{\max}} \right) \leq \ln(\sigma_o) < \ln \left((\sigma_o)_{\text{Tab}}^{K_{\max}} \right) + \Delta$$

$$\begin{aligned} f(\sigma_o, T_j) &= f \left((\sigma_o)_{\text{Tab}}^{K_{\max}}, T_j \right) \left[1 - \left(\frac{\delta_2}{\Delta} \right)^2 \right] \\ &+ f \left((\sigma_o)_{\text{Tab}}^{K_{\max}-1}, T_j \right) \left[-\frac{\delta_2}{2\Delta} + \frac{1}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \right] \\ &+ \left[\frac{\delta_2}{2\Delta} + \frac{1}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \right] \end{aligned}$$

2.8

for $j = 1, 2$ (temperature brackets)

$$\text{where } \delta_2 = \ln(\sigma_o) - \ln \left((\sigma_o)_{\text{Tab}}^{K_{\max}} \right)$$

$$\text{if } f \left((\sigma_o)_{\text{Tab}}^{K_{\max}}, T_j \right) < 1 \text{ and } f(\sigma_o, T_j) > 1 \text{ set } f(\sigma_o, T_j) = 1$$

$$\text{if } f \left((\sigma_o)_{\text{Tab}}^{K_{\max}}, T_j \right) > 1 \text{ and } f(\sigma_o, T_j) > f \left((\sigma_o)_{\text{Tab}}^{K_{\max}}, T_j \right)$$

$$\text{set } f(\sigma_o, T_j) = f\left((\sigma_o)_{\text{Tab}}^{K_{\text{max}}}, T_j\right)$$

$$5) \ln\left((\sigma_o)_{\text{Tab}}^{K_{\text{min}}}\right) + \Delta < \ln\sigma_o < \ln\left((\sigma_o)_{\text{Tab}}^{K_{\text{max}}}\right)$$

For this case $\ln(\sigma_o)$ must be located such that

$$\ln\left((\sigma_o)_{\text{Tab}}^k\right) \leq \ln(\sigma_o) < \ln\left((\sigma_o)_{\text{Tab}}^{k+1}\right)$$

Then

$$f(\sigma_o, T_j) = f_{x,k} \left[\frac{\ln\left((\sigma_o)_{\text{Tab}}^{k+1}\right) - \ln\sigma_o}{\Delta} \right] \\ + f_{x,k+1} \left[\frac{\ln(\sigma_o) - \ln\left((\sigma_o)_{\text{Tab}}^k\right)}{\Delta} \right]$$

2.9

$f_j = 1, 2$ (temperature brackets)

$$\text{where } f_{x,k} = f\left((\sigma_o)_{\text{Tab}}^k, T_j\right) \left[1 - \frac{1}{2} \left(\frac{\delta_3}{\Delta} \right)^2 \right] \\ + f\left((\sigma_o)_{\text{Tab}}^{k-1}, T_j\right) \left[-\frac{\delta_3}{2\Delta} + \frac{1}{2} \left(\frac{\delta_3}{\Delta} \right)^2 \right] \\ + f\left((\sigma_o)_{\text{Tab}}^{k+1}, T_j\right) \left[\frac{\delta_3}{2\Delta} + \frac{1}{2} \left(\frac{\delta_3}{\Delta} \right)^2 \right]$$

$$\delta_3 = \ln(\sigma_o) - \ln\left((\sigma_o)_{\text{Tab}}^k\right)$$

$$f_{x,k+1} = f\left((\sigma_o)_{\text{Tab}}^{k+1}, T_j\right) \left[1 - \frac{1}{2} \left(\frac{\delta_4}{\Delta} \right)^2 \right] \\ + f\left((\sigma_o)_{\text{Tab}}^k, T_j\right) \left[-\frac{\delta_4}{2\Delta} + \frac{1}{2} \left(\frac{\delta_4}{\Delta} \right)^2 \right] \\ + f\left((\sigma_o)_{\text{Tab}}^{k+2}, T_j\right) \left[\frac{\delta_4}{2\Delta} + \frac{1}{2} \left(\frac{\delta_4}{\Delta} \right)^2 \right]$$

$$\delta_4 = \ln(\sigma_o) - \ln\left((\sigma_o)_{\text{Tab}}^{k+1}\right)$$

3.2.3 Computation of Self-Shielding f-Factors for Specific Temperatures

The cross sections for a given material on the GMUG file are specified for at least one temperature. If temperature dependent f-factors are not supplied it will, obviously, not be necessary to carry out a temperature interpolation calculation for the material. However, a specified temperature must be included in the TDOWN input and must be in the range of temperatures for the material (see the problem example in Section 3.5). Self-shielding f-factors may be tabulated for up to three discrete values of the temperature. If TDOWN input specifies a material temperature outside the range of temperatures for that material, the code will terminate with an error flag.

It was shown in the previous section (Section 3.2.2) that the f-factor interpolation on σ_o was carried out for the two temperatures, T_j and T_{j+1} , which bracketed a specified temperature, T . The f-factor is determined by means of a simple logarithmic ratio based upon the f-factors at T_j and T_{j+1} . It is given as follows:

$$f(\sigma_o, T) = f(\sigma_o, T_j) + \frac{\ln(T/T_j)}{\ln(T_{j+1}/T_j)} \left[f(\sigma_o, T_{j+1}) - f(\sigma_o, T_j) \right] \quad 2.10$$

where T is in absolute temperature units which are consistent with the units for the T_j 's ($^{\circ}\text{K}$ or $^{\circ}\text{R}$).

The energy group material indicators and reaction type have been omitted in Equation 2.10 for convenience.

3.2.4 Computation of Self-Shielded Cross Sections

Composition and temperature dependent total, transport, fission, capture, scattering and elastic removal cross sections are determined from the appropriate f-factors and infinitely-dilute cross section values for coarse group i and material m as follows:

$$(\sigma_t)_{i,m} = f_t(\sigma_o, T)_{i,m} (\sigma_t^{\infty})_{i,m} \quad 2.11$$

$$(\sigma_{tr})_{i,m} = f_{tr}(\sigma_o, T)_{i,m} (\sigma_{tr}^{\infty})_{i,m} \quad 2.12$$

$$(\sigma_f)_{i,m} = f_f(\sigma_o, T)_{i,m} (\sigma_f^{\infty})_{i,m} \quad 2.13$$

$$(\sigma_c)_{i,m} = f_c(\sigma_o, T)_{i,m} (\sigma_c^{\infty})_{i,m} \quad 2.14$$

$$(\sigma_s)_{i,m} = f_s(\sigma_o, T)_{i,m} (\sigma_s^{\infty})_{i,m} \quad 2.15$$

$$(\sigma_{er})_{i,m} = f_s(\sigma_o, T)_{i,m} (\sigma_{er}^{\infty})_{i,m} \quad 2.16$$

The self-shielded cross sections for material m are all functions of the self-shielding parameter, σ_o , which in turn is a function of the total cross sections for the other materials in the given composition. Thus, an iterative procedure on σ_t is called for between the shielded values of the total cross sections and σ_o , as given by Equation 2.1. This iteration procedure continues only for σ_t until a maximum number of iterations, I_{max} , is reached or until the total cross section for each group and each material in a given composition satisfies the following convergence test:

$$\frac{[\sigma_t(\sigma_o^k)]_{i,m} - [\sigma_t(\sigma_o^{k-1})]_{i,m}}{[\sigma_t(\sigma_o^{k-1})]_{i,m}} < \epsilon_{ss} \quad 2.17$$

where k refers to the k -th iteration and ϵ_{ss} is an input convergence test. Following convergence, the computations in Sections 3.2.2, 3.2.3 and equations 2.11 through 2.16 are performed for the other cross sections.

3.3 Neutron Flux Solutions

Neutron flux spectra may be input or may be determined by a series of solutions in either zero or one-dimension. The flux solutions are patterned after those in the BISYN code,⁽⁵⁾ but with the fluxes computed at mid-interval rather than at interval endpoints.

The neutron spectra are primarily used to make adjustments to the elastic transfer cross sections. Since the transfer cross sections are also used in carrying out the neutron flux solutions, an iterative procedure is called for. The iterative computations will continue until the adjusted value of the elastic removal cross section satisfies a convergence test between consecutive iterations or until a maximum number of iterations has been reached.

For zero-dimensional solutions a particular composition is specified and group-dependent bucklings are input. In a more general problem, several compositions are input and linked in an x-y or R-Z arrangement.

The layout for a TDOWN example problem is shown in Figure 3 and discussed in Section 3.5. One-dimensional solutions may be performed in any given sequence of zones where the compositions are arranged as in Figure 3. In the example given, one solution is run through zones 1, 4, 5 and 7. However, one-dimensional solutions could be run in any radial rows of zones (e.g., zones 1, 2, 3 and 8) or in any axial rows of regions (e.g., regions 2, 4, 5 and 7). For the zero-dimensional arrangement of compositions and regions, a system geometry as in Figure 3 is not necessary, but may still be an aid to the user in applying TDOWN.

3.3.1 The Fission Spectrum Distribution

The fission spectrum distribution is the only other array, in addition to the elastic transfer cross sections, to be adjusted in going from one flux solution iteration to the next. Only one fission spectrum is allowed on the MUG file; however each composition used in a flux solution generates a fission spectrum according to the equation below. The fission spectrum fractions for coarse group i and for flux solution iteration $L+1$ is given as follows:

$$(\overline{\chi_i})^{L+1} = \frac{\phi_i^L \sum_m N_m \chi_{i,m} v_{i,m} (\sigma_f)_{i,m}}{\sum_i \phi_i^L \sum_m N_m \chi_{i,m} v_{i,m} (\sigma_f)_{i,m}} \quad 3.1$$

where ϕ_i^L = the neutron flux spectra for coarse group i and iteration L

$\sum_m$ = summation over all materials in the composition

and the remaining terms have the usual meanings.* After the convergence of the elastic removal cross section, the $\bar{\chi}_i$ values are determined from the last flux solution iteration and included in the multigroup output.

3.3.2 Convergence of Fluxes

The fluxes are said to be converged with respect to the elastic removal cross sections when the following conditional relationship holds for the integrated flux values,

$$\left[\begin{array}{c} \frac{\phi_{i,j}^1}{\phi_{i+1,j}^1} - \frac{\phi_{i,j}^2}{\phi_{i+1,j}^2} \\ \frac{\phi_{i,j}^2}{\phi_{i+1,j}^2} \end{array} \right] \leq \delta_c \quad 3.2$$

where $\phi_{i,j}^1$ = the flux value from the latest flux solution for the i-th coarse group and j-th region.

$\phi_{i,j}^2$ = the flux value from the previous flux solution iteration for the i-th coarse group and j-th region.

δ_c = input convergence criteria

*The fission spectrum array for the initial flux solution uses a constant flux of 1.0 for all groups i.

When Equation 4.2 is not satisfied for a particular group i and region j , and the maximum number of flux solution iterations has not been reached, the elastic removal cross sections are recomputed (see Section 3.4) and the flux solution calculations are repeated.

It is important to note that the primary use of the flux solutions is the adjustment of the elastic removal cross section through the use of the integrated flux values. Thus, internal flux solution convergence criteria (e.g., convergence on the reactivity or the fission source) can be relaxed in comparison to the normal diffusion theory type eigenvalue calculation.

3.4 Adjustments to the Elastic Removal Cross Sections

The elastic removal cross sections from the GMUG file are used in the first neutron flux solution iteration. Thereafter, the removal cross sections are determined from the general expression for isotopic scattering from the coarse group. That is for a particular region,

$$(\sigma_{er})_{i,m} \phi_i = \int_{u_i - V}^{u_i} \sigma_{s_{i,m}}(u) \phi(u)_i du \int_{u_i}^{u + \ln 1/\alpha_m} P(u \rightarrow u') du' \quad 4.1$$

where ϕ_i = The integrated flux for the i -th group

$$\phi_i = \bar{\phi}_i \Delta u$$

$P(u \rightarrow u')$ = Probability for scattering from lethargy u to lethargy u'

$$P(u \rightarrow u') = \frac{e^{(u-u')}}{1-\alpha_m}$$

V = lethargy range for scattering

$$V = \ln 1/\alpha_m \text{ if } \ln 1/\alpha_m < \Delta u_i$$

$$V = \Delta u_i \text{ otherwise}$$

$\bar{\phi}_i$ = Average flux per unit lethargy in the i-th group

and the remaining terms have the usual meanings.

Equation 4.1 can be rearranged to give the equation for the elastic removal cross section by carrying out the integration on du' , multiplying the numerator and denominator by $\xi_{i,m}(\sigma_s)_{i,m}\xi_m(u)$ and dividing both sides of the equation by $\bar{\phi}_i\Delta u_i$. Equation 4.1 then becomes

$$(\sigma_{er})_{i,m} = (\sigma_{er})_{i,m}^0 \int_{u_i-V}^{u_i} \frac{1}{\xi_m(u)} \left(\frac{\psi(u)}{\psi_{i,m}} \right) \left[\frac{e^{-(u_i-u)-\alpha_m}}{1-\alpha_m} \right] du \quad 4.2$$

where $(\sigma_{er})_{i,m}^0$ = the elastic removal cross sections for the i-th group and m-th material corresponding to a $1/E$ flux representation.

$$(\sigma_{er})_{i,m}^0 = \xi_{i,m}(\sigma_s)_{i,m}/\Delta u_i$$

$\psi(u)$ = approximation for the slowing down density, for the material being considered, as a function of lethargy

$$\psi(u) = \xi_m(u)\sigma_{s,m}(u)\phi(u)$$

$\psi_{i,m}$ = Approximation for the slowing down density of the i-th group and m-th material

$$\psi_{i,m} = \xi_{i,m}(\sigma_s)_{i,m}\bar{\phi}_i/\Delta u_i$$

All the terms in Equation 4.2 have been previously determined except for the ratio $\frac{\psi(u)}{\psi_{i,m}}$ and $\xi_m(u)$. The former term will be computed by a simple linear relationship between adjacent groups as is described in the Section 3.4.1. A similar expression could also be used for $\xi_m(u)$. However, in the present version of TDOWN it will be assumed that $\xi_m(u)$ is a slowly varying

function of lethargy and can be approximated by the groupwise value.

That is,

$$\xi_m(u) = \xi_{i,m} = \int_{u_i - \ln 1/\alpha_m}^{u_i} \frac{e^{-(u_i - u) - \alpha_m}}{1 - \alpha_m} du \quad 4.3$$

3.4.1 Variation of Slowing Down Density

The adjustments to the elastic removal cross sections are based upon an assumed linear relationship between the slowing down density and the lethargy in neighboring energy groups. This relationship is shown in the simple schematic diagram below.

The ratio of the slowing down density as a function of lethargy to the slowing down density for coarse group i is determined for two ranges of lethargy as follows:

$$a) \quad u \geq (u_i - \Delta u_i / 2)$$

$$\begin{aligned} \frac{\psi(u) - \psi_{i,m}}{\psi_{i+1,m} - \psi_{i,m}} &= \frac{u - (u_i - \Delta u_i / 2)}{(u_{i+1} - \Delta u_{i+1} / 2) - (u_i - \Delta u_i / 2)} \\ &= \frac{2(u - u_i + \Delta u_i / 2)}{(\Delta u_{i+1} + \Delta u_i)} \end{aligned} \quad 4.4$$

rearranging,

$$\frac{\psi(u)}{\psi_{i,m}} = 1 + a_{i,m} + b_{i,m} (u - u_i) \quad 4.5$$

where

$$a_{i,m} = \left(R_{i,m} - 1 \right) \left(\frac{\Delta u_i}{\Delta u_{i+1} + \Delta u_i} \right)$$

$$b_{i,m} = \left(R_{i,m} - 1 \right) \left(\frac{2}{\Delta u_{i+1} + \Delta u_i} \right)$$

$$\text{and } R_{i,m} = \xi_{i+1,m}(\sigma_s)_{i+1,m} \phi_{i+1} \Delta u_i / \xi_{i,m}(\sigma_s)_{i,m} \phi_i \Delta u_{i+1}$$

$$\text{b) } \underline{u < (u_i - \Delta u_i / 2)}$$

$$\begin{aligned} \frac{\psi_{i,m} - \psi(u)}{\psi_{i,m} - \psi_{i-1,m}} &= \frac{(u_i - \Delta u_i / 2) - u}{(u_i - \Delta u_i / 2) - (u_{i-1} - \Delta u_{i-1})} \\ &= \frac{2(u_i - \Delta u_i / 2 - u)}{\Delta u_i + \Delta u_{i-1}} \end{aligned} \quad 4.6$$

rearranging,

$$\frac{\psi(u)}{\psi_{i,m}} = 1 + a'_{i,m} + b'_{i,m} (u - u_i) \quad 4.7$$

where

$$a'_{i,m} = - \left(R'_{i,m} - 1 \right) \left(\frac{\Delta u_i}{\Delta u_i + \Delta u_{i-1}} \right)$$

$$b'_{i,m} = - \left(R'_{i,m} - 1 \right) \left(\frac{2}{\Delta u_i + \Delta u_{i-1}} \right)$$

$$\text{and } R'_{i,m} = \frac{\xi_{i-1,m}(\sigma)_{i-1,m} \phi_{i-1} \Delta u_i}{\xi_{i,m}(\sigma)_{i,m} \phi_i \Delta u_{i-1}}$$

3.4.2 Approximations for Various Degrees of Lethargy Gain

The methods to be used in correcting the elastic removal cross section are identified by the Lethargy Gain Indicator from the GMUG file and are summarized here.

$$\text{a) } \underline{\text{LGI} = 1 \quad \ln 1/\alpha_m \leq \Delta u_i/2}$$

Substituting Equation 4.5 into Equation 4.2 gives

$$(\sigma_{er})_{i,m} = (\sigma_{er})_{i,m}^0 \int_{u_i - \ln 1/\alpha_m}^{u_i} \frac{1}{\xi_m(u)} (1 + a_{i,m} + b_{i,m}(u - u_i)) \left[\frac{e^{-(u_i - u) - \alpha_m}}{1 - \alpha_m} \right] du \quad 4.8$$

Replacing $\xi_m(u)$ by the expression in Equation 4.3 and carrying out the integration results in the following equation for the removal cross section:

$$(\sigma_{er})_{i,m} = (\sigma_{er})_{i,m}^0 \left[1 + a_{i,m} + b_{i,m} \left(\frac{\alpha_m (\ln \alpha_m)^2}{2 \xi_{i,m} (1 - \alpha_m)} - 1 \right) \right] \quad 4.9$$

where $a_{i,m}$ and $b_{i,m}$ are defined for Equation 4.5.

$$\text{b) } \underline{\text{LGI} = 2 \quad (\Delta u_i/2 < \ln 1/\alpha \leq \Delta u_i)}$$

Substituting Equations 4.5 and 4.7 into Equation 4.2 gives

$$\begin{aligned} (\sigma_{er})_{i,m} = (\sigma_{er})_{i,m}^0 & \left\{ \int_{u_i - \Delta u_i/2}^{u_i} \frac{1}{\xi_m(u)} (1 + a_{i,m} + b_{i,m}(u - u_i)) \left[\frac{e^{-(u_i - u) - \alpha_m}}{1 - \alpha_m} \right] du \right. \\ & \left. + \int_{u_i - \ln 1/\alpha}^{u_i - \Delta u_i/2} \frac{1}{\xi_m(u)} (1 + a'_{i,m} + b'_{i,m}(u - u_i)) \left[\frac{e^{-(u_i - u) - \alpha_m}}{1 - \alpha_m} \right] du \right\} \quad 4.10 \end{aligned}$$

Replacing $\xi_m(u)$ by $\xi_{i,m}$ and carrying out the integration results in the following equation for the removal cross section:

$$\begin{aligned}
 (\sigma_{er})_{i,m} = \frac{(\sigma_{er})_{i,m}^0}{\xi_{i,m}(1-\alpha_m)} & \left\{ (1+a_{i,m}) \left[1 - \alpha_m \frac{\Delta u_i}{2} - e^{-\Delta u_i/2} \right] \right. \\
 & - b_{i,m} \left[1 - \frac{1}{8}\alpha_m \Delta u_i^2 - \left(1 + \frac{\Delta u_i}{2} \right) e^{-\Delta u_i/2} \right] \\
 & + (1+a'_{i,m}) \left[e^{-\Delta u_i/2} - \alpha_m \left(1 - \frac{\Delta u_i}{2} - \ln \alpha_m \right) \right] \\
 & \left. + b'_{i,m} \left[\alpha_m (1 - \ln \alpha_m - \frac{1}{8}\Delta u_i^2 + \frac{1}{2}\ln^2 \alpha_m) - \left(1 + \frac{\Delta u_i}{2} \right) e^{-\frac{\Delta u_i}{2}} \right] \right\} \quad 4.11
 \end{aligned}$$

where $a_{i,m}$ and $b_{i,m}$ are defined for Equation 4.5 and $a'_{i,m}$ and $b'_{i,m}$ are defined for Equation 4.7.

c) LGI = 3 $\ln 1/\alpha > \Delta u_i$

Substituting Equations 4.5 and 4.7 into Equation 4.2 gives

$$\begin{aligned}
 (\sigma_{er})_{i,m} = (\sigma_{er})_{i,m}^0 & \left\{ \int_{u_i - \Delta u_i/2}^{u_i} \frac{1}{\xi_m(u)} (1+a_{i,m}+b_{i,m}(u-u_i)) \left[\frac{e^{-(u_i-u)-\alpha_m}}{1-\alpha_m} \right] du \right. \\
 & \left. + \int_{u_i - \Delta u_i}^{u_i - \Delta u_i/2} \frac{1}{\xi_m(u)} (1+a'_{i,m}+b'_{i,m}(u-u_i)) \left[\frac{e^{-(u_i-u)-\alpha_m}}{1-\alpha_m} \right] du \right\} \quad 4.12
 \end{aligned}$$

Replacing $\xi_m(u)$ by $\xi_{i,m}$ and carrying out the integration results in the following equation for the removal cross section:

$$\begin{aligned}
(\sigma_{er})_{i,m} = \frac{(\sigma_{er})_{i,m}^0}{\xi_{i,m}(1-\alpha_m)} \left\{ (1+a_{i,m}) \left[1 - \alpha_m \frac{\Delta u_i}{2} - e^{-\Delta u_i/2} \right] \right. \\
- b_{i,m} \left[1 - \frac{1}{8} \alpha_m \Delta u_i^2 - (1 + \Delta u_i/2) e^{-\Delta u_i/2} \right] \\
+ (1 + a'_{i,m}) \left[e^{\frac{\Delta u_i}{2}} - e^{-\Delta u_i} - \alpha_m \Delta u_i/2 \right] \\
\left. + b'_{i,m} \left[(1+\Delta u_i) e^{-\Delta u_i} - (1+\Delta u_i/2) e^{-\Delta u_i/2} + 3/8 \alpha_m \Delta u_i^2 \right] \right\} \quad 4.13
\end{aligned}$$

where $a_{i,m}$ and $b_{i,m}$ are defined for Equation 4.5 and $a'_{i,m}$ and $b'_{i,m}$ are defined for Equation 4.7.

3.4.3 Elastic Removal for Hydrogen

For the special case of scattering from hydrogen, the elastic removal cross section in Equation 4.2 is modified as follows:

$$(\sigma_{er})_{i,H} = \frac{(\sigma_{er})_{i,H}^0}{1 - e^{-\Delta u_i}} \int_{u_i - \Delta u_i}^{u_i} \left(\frac{\psi(u)}{\psi_{i,H}} \right) e^{-(u_i - u)} du \quad 4.14$$

where $(\sigma_{er})_{i,H}^0$ is defined as in Appendix B by

$$(\sigma_{er})_{i,H}^0 = \frac{(\sigma_s)_{i,H}}{\Delta u_i} (1 - e^{-\Delta u_i})$$

and α_H and $\xi_{i,H}$ are 0 and 1 respectively.

Substituting Equations 4.5 and 4.7 into Equation 4.14 gives

$$\begin{aligned}
(\sigma_{er})_{i,H} = (\sigma_{er})_{i,H}^0 & \left\{ \int_{u_i - \Delta u_i / 2}^{u_i} (1 + a_{i,H} + b_{i,H}(u - u_i)) e^{-(u_i - u)} du \right. \\
& \left. + \int_{u_i - \Delta u_i}^{u_i - \Delta u_i / 2} (1 + a'_{i,H} + b'_{i,H}(u - u_i)) e^{-(u_i - u)} du \right\} \quad 4.15
\end{aligned}$$

Carrying out the integration results in the following equation for the removal cross section for hydrogen:

$$\begin{aligned}
(\sigma_{er})_{i,H} = \frac{(\sigma_{er})_{i,H}^0}{(1 - e^{-\Delta u_i})} & \left\{ (1 + a_{i,H}) \left[1 - e^{-\Delta u_i / 2} \right] \right. \\
& - b_{i,H} \left[1 - \left(1 + \Delta u_i / 2 \right) e^{-\Delta u_i / 2} \right] \\
& + (1 + a'_{i,H}) \left[e^{-\Delta u_i / 2} - e^{-\Delta u_i} \right] \\
& \left. + b'_{i,H} \left[e^{-\Delta u_i} (1 + \Delta u_i) - e^{-\Delta u_i / 2} \left(1 + \frac{\Delta u_i}{2} \right) \right] \right\} \quad 4.16
\end{aligned}$$

where $a_{i,H}$ and $b_{i,H}$ are defined for Equation 4.5 and $a'_{i,H}$ and $b'_{i,H}$ are defined for Equation 4.7.

3.4.4 Adjustment of the Elastic Matrix

The elastic matrix terms, if included in the GMUG file (optional), are specified as functions which sum to 1.0. That is,

$$\sum_{\ell=i+1}^{L_{\max}} g_{i \rightarrow \ell, m} \quad (1 \leq i \leq I_{\text{tot}} - 1) \quad 4.17$$

where $g_{i \rightarrow \ell}$ = the fraction of the neutrons which are elastically scattered from group i to group ℓ for the m -th material

I_{tot} = total number of energy groups

$L_{\text{max}} = i + L_{\text{scat}}$ or I_{tot} whichever is smaller

L_{scat} = a specified maximum number of downscatter groups

The elastic matrix cross sections for the output MUG file are determined by multiplying the adjusted removal cross section (or the removal cross section from the GMUG file which is used for the first iteration of the neutron flux solutions) by the elastic transfer fractions as follows,

$$(\sigma_{\text{er}})_{i \rightarrow l, m} = (\sigma_{\text{er}})_{i, m} g_{i \rightarrow l, m} \quad 4.18$$

for $(1 \leq i \leq I_{\text{max}} - 1)$

$(l = i+1 \text{ to } L_{\text{max}})$

3.5 Example Problem for TDOWN

For purposes of illustrating the use of the TDOWN code, a hypothetical TDOWN problem is described in this section.

Consider the reactor description shown in Figure 3, which corresponds to typical flux solution problem to be run after TDOWN. The core, radial blanket and axial blanket are each divided into two zones, with both zones having the same basic composition but different fissile enrichments. The axial reflector composition is also different from the radial reflector.

In setting up the TDOWN problem, the user must decide which cross section modifications are to be applied to each material in each zone. A full-blown problem would have the self-shielding correction applied to each material in each separate composition and the flux spectrum modification applied for each material in each zone. Retaining such detail

FIGURE 3

REACTOR DESCRIPTION* FOR HYPOTHETICAL TDOWN PROBLEMS

1-D Flux Solution
 (Flux Set 1 for core zone-input)

*Only U-238 and Fe materials are described for the compositions. Descriptions of other materials are not needed for this illustration.

**In this example, compositions 2 and 4 represent composition 1 and 2 at different temperatures. However, they are additional compositions independent of any zone - they would not be included in the zonal (regional) description in TDOWN input.

in this problem is totally out of balance with the accuracy of the rapid cross section adjusting approach, itself, and the burden of carrying it along in subsequent computations would be crippling. Thus, the user should judiciously choose which materials must be modified in which compositions and spectra. Considering just U-238 and Fe in this problem will illustrate this point.

U-238 is present in zones 1 through 6, in Figure 3, but in varying amounts. Since self-shielding of U-238 is important in the analysis, separate output cross section sets for U-238 in each of the core zones and the axial and radial blankets will be required (a total of 4), considering the self-shielding modification only. Neutron moderation by U-238 is not extensive, so the spectral modification to elastic removal needs to be done only for a spectrum representative of the core, and one representative of both blankets.

Iron is present in all zones of the reactor, with approximately the same concentration in zones 1 through 6. For purposes of illustration, let us say that the axial and radial reflectors have relatively high concentrations of Fe. Since self-shielding of Fe in the core and blankets is not of major concern, a set of Fe output cross sections for zones 1 through 6 and another for zones 7 and 8 are all that are required from consideration of self-shielding alone. However, spectral effects on Fe are important and the difference between spectra in the core, blankets and reflectors must be considered. Thus a separate output cross section set will be needed for iron in each of these three major regions.

To obtain the spectra for the elastic removal modification, the user has the choice of putting them in from cards, if suitable spectra are available, or computing them by zero- or one-dimensional diffusion theory solutions. In this case, assume the user has a good representative spectrum for the core but not for the blankets and reflectors. To get the latter two spectra, a one-dimensional solution will be run axially through zones 1, 4, 5 and 7, with the proper radial bucklings input. The spectra taken from this solution will then be those in zones 4 and 7.

One other consideration to be made is that of temperature effects. In order to compute a Doppler coefficient, U-238 cross section sets for both core zones must be output for two different U-238 temperatures. This is accomplished by repeating the compositions in core zones 1 and 2 as

additional composition sets, but with U-238 at the second temperature.

Specification of the U-238 and Fe output cross section sets will then be the following:

<u>Output File Material No.</u>	<u>GMUG Material No.</u>	<u>Temperature</u>	<u>Composition Set No.</u>	<u>Flux Set No.</u>
381	1103	1400	1	1
382	1103	700	2	1
383	1103	1400	3	1
384	1103	700	4	1
385	1103	1000	5	2
386	1103	1000	6	2
261	1122	900	1	1
262	1122	900	5	2
263	1122	900	7	3

The zone and assignments of the output file material numbers for U-238 and Fe are indicated in Figure 3. The corresponding composition and flux set numbers are given by the following:

<u>Composition Set No.</u>	<u>Source</u>	<u>Flux Set No.</u>	<u>Source</u>
1	Zone 1 U-238 at 1400°	1	Input for core
2	Zone 1 U-238 at 700°	2	Zone 4 from Flux Solution
3	Zone 2 U-238 at 1400°	3	Zone 7 from Flux Solution
4	Zone 2 U-238 at 700°		
5	Zone 4,5		
6	Zone 6		
7	Zone 7		

SECTION IV

PROGRAM DESCRIPTION

The TDOWN program contains a main controlling routine and ten links. The links are logical division of the coding and they are used to minimize the memory requirements of the code. Links may be overlaid so that data processing is carried out with only the necessary coding instructions in the computer.

The broad program logic and the purpose of each link are illustrated in Figure 4. In the illustration some links have two names; the second name specifies the link overlaid by the first. Following Figure 4 is a brief description of the MAIN program and each link.

FIGURE 4

MAIN

- The MAIN routine directs the sequential execution of the code computations and contains the blank and labeled common used for transferring data from link to link. Also included in MAIN are the subroutines which store and retrieve data. These subroutines are not overlaid and are called and used by other links.

TDL1

- A set of Generalized Input Program routines are contained in this link. These routines interpolate the input data and store it in specified classes for use in later computations.

COMMON

- Peripheral devices for Input/Output and scratch files are defined in this link. Also several general purpose service routines are loaded for use by the other links.

BUFFER

- The routine in BUFFER sets up an area of blank common for working space.

TDL2

- Initial calculations are carried out using the input data. At the same time the input is edited and checked for consistency and completeness. The required data from the GMUG file is processed and transferred onto working files.

TDL3

- The microscopic cross sections are calculated by routines in TDL3. Calculations include the determination of the self-shielding parameters, σ_0 's, and the f-factor interpolation on temperature and σ_0 . The cross section computation is carried out by iterative procedure.

- Neutron flux solutions in the fundamental mode or one-dimension are carried out in link TDL4. The principal sub-links in this overlay are named and described below:

TDL4A - Macroscopic cross sections are computed for all compositions used in a flux solution.

TDL4B - Zero or one-dimensional diffusion calculations are carried out in TDL4B.

TDL4C - The elastic removal cross sections are adjusted for the energy distribution of the neutron flux spectra.

TDL5

- In this link, elastic removal cross sections are corrected for all materials in compositions not included in any flux solution. If fluxes were input the χ_i (fraction of fission neutrons in group i) can be calculated in this link.

TDL6

- This link contains the routine for writing the MUG file tape. Prior to transferring the data to tape the matrices are combined into the inelastic matrix which may be reduced depending on the input specifications.

TDL7

- The code edits as specified in CLASSES 9 and 19 of the input are written by the routines in this link.

LAST

- The program is ended with this link. All files are closed and rewound.

SECTION V

INPUT DESCRIPTION

The input description for TDOWN given here includes both control cards required for execution of the code on the GE-635 computer and the data cards for a TDOWN case.

5.1 Control Cards for Running on the GE-635 Computer

<u>Card Purpose</u>	<u>Contents</u>		
	Column: <u>1</u>	<u>8</u>	<u>16</u>
Job identification	\$	IDENT	CCCC,III-locat,TDOWN
Program loader	\$	PROGRAM	RLHS
Program Limits	\$	LIMITS	tt,32K,10K,10000
TDOWN program	\$	TAPE	H*,H1DD,,MMM,,TD-CODE
GMUG file	\$	TAPE	01,G1DD,,MMM,,GMUG File
MUG file	\$	TAPE	02,M1DR,,,MUG FILE
Peripheral storage	\$	FILE	10,,5R
Peripheral storage	\$	FILE	11,,5R
Peripheral storage	\$	FILE	12,,50R
Peripheral storage	\$	FILE	13,,5R
Peripheral storage	\$	FILE	14,,5R
Peripheral storage	\$	FILE	15,,15R
Output file - printed	\$	SYSOUT	P*
Output file - printed	\$	SYSOUT	06
Output file - printed	\$	SYSOUT	33
Transliteration	\$	INCODE	IBMF
			(Data Cards)
Conclusion of Job	\$	ENDJOB	

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

TAPE, FILE and SYSOUT files all have alphanumeric file code numbers in columns 16 and 17. These numbers are used in the program to reference the separate peripheral storage devices.

Following the double commas on the FILE cards are the number of 3840 word links (nR) available for storage on each peripheral unit. The TDOWN FILE size requirements can be calculated by recipe. However, the number of links shown on the files should be more than adequate for most problems.

5.2 Data Cards

The data cards are inserted between the transliteration (INCODE) and conclusion (ENDJOB) cards.

A. CASE and LAST cards

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

Card Column:	1	28
CASE card	)TDWNiii*cccc	dddddd
Data Cards		
LAST card	)LAST	

iii = user's initials	}	optional
cccc = case name		
dddddd = date		

B. SIZE Card

The SIZE card defines the computer memory requirements of the problem. TDOWN is variably dimensioned, consequently the input parameters listed below do not have definite size limits. However, some of the parameter sizes are limited due to other linked codes and to avoid excessive core

requirements practical limits are given for the input parameters below.

The SIZE card must follow the CASE card.

<u>Card Columns</u>	<u>Contents</u>
33-35	ITOT - Number of lethargy groups (integer) $1 \leq \text{ITOT} \leq 100$
38-40	MTPC - Number of compositions (integer) $1 \leq \text{MTPC} \leq 100$
43-45	MMPC - Maximum number of materials (integer) $1 \leq \text{MMPC} \leq 120$
49-50	NREGX* - Number of regions in x-direction (integer) $1 \leq \text{NREGX} \leq 20$
54-55	NREGY* - Number of regions in y-direction (integer) $1 \leq \text{NREGY} \leq 20$
58-60	NFSET - Total number of flux sets (integer) $0 \leq \text{NFSET} \leq 100$
64-65	NFSOL - Total number of flux solutions (integer) $0 \leq \text{NFSOL} \leq 10$

C. WRAPUP-RESTART Card

At present no wrapup or restart capabilities are available in TDOWN. However, a blank card must follow the problem size information card.

D. CLASS cards

The following description will be the general format found on all CLASS (data) cards. Rules governing the variable style (NIPS) input format will also be discussed. Note: Numbers discussed in columns 1-20 must always be right justified in their respective columns.

*On the SIZE card only, these variables must be > 0 even if the problem doesn't require a geometry description.

1. General Format of CLASS Cards

<u>Column</u>	<u>Definition</u>
1-3	CLASS number
4-6	Record number
7-9	I, loading index of first value in data field (this index is either the first dimension of a multi-dimensional array or it may be the computed algorithm $I + \text{IMAX}*(J-1) + \text{IMAX}*J\text{MAX}*(K-1)$ etc.)
10-12	J, 2nd index of a two- or three-dimensional array.
13-15	K, 3rd index of a three-dimensional array.
16-17	Repeat option, defined as follows:
IR	Record insert: all data for this record will be inserted in record L (Col. 18-20)
IJ	J insert: all values for $N=J$ will be inserted for $J=L$.
IK	K insert: all values for $K=K$ will be inserted for $K=L$.
RR	Record repeat: repeat this record through record L.
NOTE:	<u>The four options above cause columns 21-80 to be ignored.</u>
RJ	J repeat: repeat the values on this card for all locations J through L.
RK	K repeat: repeat the values on this card for all locations K through L.
RO	Record overlay: values on this card will be loaded for this record through record L.
18-20	L, termination index of option in Columns 16-17.
21-80	Input data using NIPS format.

2. NIPS Format (Variable Format)

2a. Only 20 characters have any meaning; they are:

+ - . 0 1 2 3 4 5 6 7 8 9 E H R S () \$

All other characters are interpreted as a blank, and will be denoted by the symbol Δ .

2b. One or more Δ 's are used to separate entities and may be in the form of a blank, comma, etc.

2c. Numerical data have the usual configuration.

Integer: Δ (optional sign) (sequence of digits)

*Floating point: Δ (optional sign) (sequence of digits with one decimal point)

Scaled floating point: (floating point) (optional E) (sign) (sequence of digits).

2d. BCD (Hollerith) data must always be preceded by the number of BCD characters and an H followed by the BCD data. $\Delta 6HXXXXXX$.

2e. Repeat loading of a word may be accomplished by following the word with $\Delta Rnnn$ where nnn is a positive integer (not preceded by a Δ) representing the number of times the word is loaded.

2f. Skipping location(s) is accomplished by entering the configuration $\Delta Snnn$, where nnn is a positive integer (not preceded by a Δ) representing the number of locations to be skipped.

2g. Comments may be mixed with data by entering a Δ (before the comments. Parentheses may be included within the comments; the comments are terminated by the) which is associated (in the usual sense) with the first left parenthesis. If the complete card is to be used as a comment card then columns 1-20 must be identical to either the preceding data card or the following data card so the comment card will not be rejected as an invalid input card.

*A floating point number must have a decimal point punched in the input card or it will be interpreted as an integer.

All of the input CLASSES described later are not necessary for every TDOWN case. Deck setups for the simplest case and cases selecting optional calculations are shown here.

(a). Case with all neutron flux spectra input.

Required CLASSES include:

1. CLASS 2 General Data
2. CLASS 5 Material Numbers and their Nuclear Density
3. CLASS 32 Material Definitions
4. CLASS 34 Input Flux Sets
5. CLASS 999

Optional CLASSES include:

1. CLASS 9 Edit options
2. CLASS 19 Edit Specifications for CLASS 9
3. CLASS 35 Cell Dimensions for Heterogeneity Correction
4. CLASS 36 Fission Fractions for Compositions

(b). Case with a Zero or One-dimensional Flux Solution

Required CLASSES include:

1. CLASS 2 General Data
2. CLASS 3 Geometry Data
3. CLASS 4 Buckling Data
4. CLASS 5 Material Numbers and their Nuclear Density
5. CLASS 6 Boundary Condition Sets
6. CLASS 7 Flux Solution Data
7. CLASS 8 Composition Map
8. CLASS 17 Region Data for Flux Solutions
9. CLASS 32 Material Definitions
10. CLASS 999

Optional CLASSES include:

1. Same as those for (a)
2. CLASS 34 Input flux sets (these sets would be in addition to those calculated by flux solution)

CLASS 2 - General Data (Always required)

<u>Columns</u>	<u>Content</u>
3	2
6	1
7-9	Starting location for loading first data value on card.
21-80	Data

<u>Starting Location</u>	<u>Content</u>
1	ITOT - Number of lethargy groups on GMUG file (integer)
2	NTDC - Number of material compositions (integer)
3	NREGX - Number of regions in the x-direction (integer)
4	JEOMX - Geometry indicator for the x-direction (integer) 0 = slab geometry 1 = cylindrical geometry 2 = spherical geometry
5	NREGY - Number of regions in the y-direction (integer)
6	JEOMY - Geometry indicator for the y-direction (see 4 above) (integer)
7	RADX - Distance (cm) from a reference line to the left interface of the first region in the x-direction (floating point)
8	RADY - Distance (cm) from a reference line to the bottom interface of the first region in the y-direction (floating point)
9	STEMP - Core temperature ($^{\circ}$ K) (floating point)
10	LIMSS - Iteration limit for determining σ_0 in self-shielding calculation (integer)
11	DELSS - Convergence criteria for self-shielding calculation (floating point)

<u>Starting Location</u>	<u>Content</u>
12	IFHET - Heterogeneity indicator (integer) 0 = all compositions are homogeneous 1 = at least one composition is heterogeneous
13	IDMUG - MUG file name (Hollerith - 5 alphanumeric characters)
14	MLGP - Highest numbered MUG file group to have an inelastic scattering matrix (integer)
15	MDS - Number of groups any group may downscatter in MUG file (integer)
16	ICHI - Composition number to use for χ_i values on the MUG file (integer)
17	KFLUX - Flux set number to be used in calculating the MUG file χ_i values (integer)
18-63	Not used
64	ICHECK - Indicator for input check Set to 1 for input checking only; the input data will be processed and edited but no calculations will be carried out.

CLASS 3 - Geometry Data (Not required if all flux sets are input)

<u>Column</u>	<u>Content</u>
3	3
6	1 = geometry for x-direction 2 = geometry for y-direction
7-9	Starting location of first data value on card.
21-80	Data - $m_1, R_1, m_2, R_2, \dots, m_k, R_k$, where: m = number of mesh <u>intervals</u> in Region k for indicated direction (integer) and R = distance (cm) from reference point to the top or right boundary of Region k for indicated direction (floating point) <u>Do not</u> count m and R as pairs for the purpose of columns 7-9.

CLASS 4 - Buckling Sets (Required only for flux solutions)..

<u>Column</u>	<u>Content</u>
3	4
6	Buckling set number. (A maximum of 20 sets is allowed)
7-9	i, the group number for the first buckling value on the card
21-80	Data - Bucklings (cm^{-2}) (floating point).

CLASS 5 - Material Numbers and their Nuclear Density (always required)

<u>Column</u>	<u>Content</u>
3	5
6	1
7-9	Starting location for loading first material number and its nuclear density. (maximum of 40 materials per composition is allowed)
10-12	Composition number
21-80	Data - $m, N_m, m, N_m, \dots$

where:

m = material number, (integer) and

N_m = nuclear density (nuclei/barn-cm) of that material in this composition (floating point)

Do not count m and N_m as pairs for columns 7-9.

CLASS 6 - Boundary Condition Sets (Required only for flux solutions)

<u>Column</u>	<u>Content</u>
3	6
6	Boundary condition set number. (A maximum of 5 sets is allowed)
7-9	i, the group number of the first value on the card.
21-80	Data - Boundary condition values (floating point)

CLASS 7 - Flux Solution Data (Required only for flux solutions)

<u>Column</u>	<u>Content</u>
3	7
6	Solution number (numbered sequentially)
7-9	i, the starting location (for this solution) of the first value on the card
12	1
21-80	Data

<u>Starting Location</u>	<u>Content</u>
--------------------------	----------------

Starting locations define the type of flux solution (0 or 1-dimensional) and specify which regions are involved. For a 0-D solution both x and y must be specified. For a 1-D solution, x = region index for a y-directed solution and y = 0. Similarly, y = region index for a x-directed solution and x = 0.

1	x-direction region (integer)
2	y-direction region (integer)
3	Maximum number of acceleration cycles (integer)
4	Number of iterations per acceleration cycle (integer)
5	Maximum number of flux iterations (integer)
6	Leakage change cycle (integer)
7	Boundary condition set number for left or bottom boundary (integer)
8	Boundary condition set number for right or top boundary (integer)
9	First mesh interval to check fission source convergence (integer)
10	Last mesh interval to check fission source convergence (integer)

<u>Starting Location</u>	<u>Content</u>
11	Option to check for negative total removal cross section (integer) 0= do not check 1= flag but do not alter 2= flag and set all negative total removal cross sections to 0.0
12	Option indicates course of action to be taken if negative fluxes are encountered (integer) 0 = error exit 1 = set all negative total removal cross sections to 0.0 and re-try solution 2 = set those negative bucklings to 0.0 for which the fluxes were negative or if word 11 above = 2, set the negative bucklings = 0.0 for those groups which the total removal cross section was negative.
13-16	Not used
17	Leakage probability (fraction) in direction of calculation (floating point)
18	Second mode leakage probability (fraction) (floating point)
19	Ratio of second mode buckling to first (floating point)
20	Convergence criterion for Δk (floating point)
21	Convergence criterion on the fission source (floating point)
22	Convergence criterion on the group fluxes (floating point)

CLASS 8 - Composition Map (only those compositions included in a flux solution need be in this CLASS)

<u>Columns</u>	<u>Content</u>
3	8
6	1
7-9	i, x-direction region index for the first value on the card
10-12	j, y-direction region index for the values on the card
21-80	Data - composition numbers to be applied to regions (i,j) (integer)

CLASS 9 - Edit Options (always required)

<u>Columns</u>	<u>Content</u>
3	9
6	1
7-9	Starting location for loading first data value on card
21-80	Data - No edit of a data type will be done if starting location value = 0

<u>Starting Location</u>	<u>Content</u>
1	1 = edit input data
2	1 = edit σ_0 , self-shielding cross section, for all materials 2 = edit σ_0 , for materials specified by CLASS 19
3	1 = edit microscopic cross sections for all materials 2 = edit microscopic cross sections for materials specified by CLASS 19
4	Not used
5	1 = edit complete MUG file
6-8	Not used
9	1 = edit flux sets generated in all flux solutions 2 = edit flux sets specified in CLASS 19

<u>Starting Location</u>	<u>Content</u>
10	1 = edit macroscopic cross sections for all compositions 2 = edit macroscopic cross sections for compositions specified in CLASS 19
11	1 = edit flux history

CLASS 17 - Region Data for Flux Solutions (required only for flux solutions)

<u>Column</u>	<u>Content</u>
2-3	17
6	Record, flux solution number
7-9	i, beginning region index (indices are numbered sequentially starting with left or bottom region depending on whether it is a x or y directed solution)
12	j = 1, data is the flux set number for regional fluxes generated by the flux solution - if a zero number is assigned to a regional flux set, the set will not be saved for use in the remaining calculations. j = 2, data is the orthogonal buckling set number to be used in this region in the flux solution j = 3, data is the third-dimensional buckling set number to be used in this region in the flux solution
21-80	Data - depending on j in column 12

CLASS 19 - Edit Specifications for CLASS 9 Data Types (always required)

<u>Column</u>	<u>Content</u>										
2-3	19										
6	Record, corresponds to starting location in CLASS 9 having a value 2.										
9	Starting location for loading first data value on cards										
21-80	Data - depending on record (integer)										
	<table> <tr> <th><u>Record Number</u></th><th><u>Data</u></th></tr> <tr> <td>2</td><td>Specify material numbers</td></tr> <tr> <td>3</td><td>Specify material numbers</td></tr> <tr> <td>9</td><td>Specify flux set numbers</td></tr> <tr> <td>10</td><td>Specify composition numbers</td></tr> </table>	<u>Record Number</u>	<u>Data</u>	2	Specify material numbers	3	Specify material numbers	9	Specify flux set numbers	10	Specify composition numbers
<u>Record Number</u>	<u>Data</u>										
2	Specify material numbers										
3	Specify material numbers										
9	Specify flux set numbers										
10	Specify composition numbers										

CLASS 32 - Material Definitions (always required)

<u>Column</u>	<u>Content</u>
2-3	32
6	1
7-9	Starting location for loading first data value on card
10-12	j, material count
21-80	Data

<u>Starting Location</u>	<u>Content</u>
1	MUG material number, m, designated in CLASS 5 (integer)
2	GMUG material number for material (integer)
3	Temperature ($^{\circ}$ K) of material (The temperature must be in the range of temperatures given for the GMUG material. If it is not input here, the temperature input in CLASS 2 will be used.) (floating point)

<u>Starting Location</u>	<u>Content</u>
4	Reference composition for determining self-shielding cross section of the material (integer)
5	Flux set number to be used in correcting σ_{er} for the material (0 = no correction to σ_{er}) (integer)
6-7	Not used
8	Indicator for heterogeneity correction: 0 = do not correct material for heterogeneity effects; 1 = perform heterogeneity correction for a cylindrical cell 2 = perform heterogeneity correction for a slab cell (integer)
9	Fraction of material in inner region if heterogeneity correction is indicated (floating point)

CLASS 34 - Input Flux Sets (Required only if flux sets are input)

<u>Column</u>	<u>Content</u>
2-3	34
6	Record, flux set number
7-9	i, the group number for the first flux value on card
21-80	Data - Integrated fluxes by group (arbitrary normalization)

CLASS 35 - Cell Dimensions for Heterogeneity Correction (This class is required for every composition having a heterogeneous treatment of materials as defined by the CLASS 32 data.)

<u>Column</u>	<u>Content</u>
2-3	35
6	1
7-9	Starting location of first value on card

<u>Column</u>	<u>Content</u>
10-12	j, composition number
21-80	Data

<u>Starting Location</u>	<u>Content</u>
1	Diameter (cylindrical) or thickness (slab) (in cm) of the inner cell region, D_1 .
2	Diameter (cylindrical) or thickness (slab) (in cm) of the outer cell region, D_2 . For definitions of D_1 and D_2 , see Figure 2.

CLASS 36 - Fission Fractions for Compositions (The fission fractions
will be calculated if they are not input.)

<u>Column</u>	<u>Content</u>
2-3	36
6	Record, composition number to use fission fractions
7-9	i, the group number of the first value on the card.
21-80	Fission fraction values (floating point)

CLASS 999 Must be the card preceding the LAST card

<u>Column</u>	<u>Content</u>
1-3	999

SECTION VI

GLOSSARY OF SYMBOLS

D_1	The inner dimensions of a cell or plate
D_2	The outer dimensions of a cell or plate
E_i	Lower energy value of group i
f_n	The fraction of the n-th material in a region
$f(\sigma_o, T)$	The f-factor at a specific σ_o and temperature
$g_{i \rightarrow l, m}$	The fraction of neutrons which are elastically scattered from group i to group l for the m-th material
N_m	Nuclear density of material m (nuclei/barn-cm)
$P(u \rightarrow u')$	Probability for scattering from lethargy u to lethargy u'
T	Material temperature ($^{\circ}K$)
T_j	Temperature for which f-factors are tabulated ($^{\circ}K$ or $^{\circ}F$)
u_i	The highest lethargy value of group i
V	Lethargy range for scattering
α_m	Ratio of final to initial neutron energy in maximum energy loss elastic collision for material m
δ_c	Input convergence criteria for fluxes
ϵ_{ss}	Input convergence criteria for σ_o
Δ	The logarithmic decrement between the consecutive values of σ_o
Δu_i	Lethargy width of group i
$\nu_{i, m}$	Average number of neutrons produced per fission of material m in energy group i

$\xi_m(u)$	The value of $\xi_{m,i}$ evaluated over the lethargy range from which neutrons may be scattered from an energy group
$\xi_{m,i}$	The average value of the logarithmic energy decrement for energy group i
σ_c	Capture cross section
σ_{er}	Elastic removal cross section
σ_f	Fission cross section
σ_{sh}	Scattering cross section for hydrogen
σ_t	Total cross section
σ_{tr}	Transport cross section
$(\sigma_x^\infty)_{i,m}$	The infinite dilute cross section for material m, group i and reaction x
$(\sigma_o)_{i,m}$	The parameter representing the total cross section of "other materials" used for specifying the degree of resonance self-shielding for material m, energy group i
$(\Sigma_{SG})_i$	The Selengut-Goertzel removal cross section
$\bar{\phi}_i$	Average flux in per unit lethargy in the i-th group
$\phi_{i,j}$	Integral flux for energy group i, region j
χ_i	Fraction of fission neutrons with energies within energy group i
$\psi(u)$	Approximation for the slowing down density as a function of lethargy
$\psi_{i,m}$	Approximation for the slowing down density of the i-th group and m-th material

SECTION VII

SAMPLE PROBLEM

7.1 Description

The computer output for a sample problem is given in this section. The problem generated 29 group cross sections for an assembly consisting of 5 regions containing 5 compositions. A one-dimensional flux solution was specified in the radial direction to generate the flux sets used to correct the elastic removal cross sections.

7.2 Output

The output listing for the sample problem include:

- a) a listing of the input class cards.
- b) an edit of the input summarizing the problem specifications
- c) the geometry in both the x and y directions
- d) description of the flux solution
- e) a description of the compositions
- f) the flux solution history for each iteration
- g) the flux sets showing integrated flux values and plots
- h) the MUG file generated consisting of:
 - 1) the χ_i and Δu_i values for each group
 - 2) the cross sections for each material as it appears on the MUG file; first the scattering matrices, second, the group average cross sections
- i) the self-shielded cross section, σ_0 , for each material

Several pages of the output have been deleted to conserve space. The listing that is included does represent all of the types of output available from this problem.*

* Special output for use by the programmer was obtained by setting indicators in words 19 and 20 in CLASS 9. This output type is not included in the report.

32	1	1	17	1	0	204	1104	300	2	2	\$
32	1	1	18	1	0	205	1105	300	2	2	\$
32	1	1	19	1	0	206	1106	300	2	2	\$
32	1	1	20	1	0	205	1055	300	2	2	\$
32	1	1	21	1	0	202	1102	300	2	2	\$
32	1	1	22	1	0	203	0103	300	2	2	\$
32	1	1	23	1	0	240	1140	300	2	2	\$
32	1	1	24	1	0	213	1013	300	2	2	\$
32	1	1	25	1	0	259	1059	300	2	2	\$
32	1	1	26	1	0	215	1015	300	2	2	\$
32	1	1	27	1	0	222	1122	300	2	2	\$
32	1	1	28	1	0	221	1121	300	2	2	\$
32	1	1	29	1	0	223	1123	300	2	2	\$
32	1	1	30	1	0	219	1019	300	2	2	\$
32	1	1	31	1	0	287	1087	300	2	2	\$
32	1	1	32	1	0	211	1111	300	2	2	\$
32	1	1	33	1	0	302	1102	300	3	3	\$
32	1	1	34	1	0	303	0103	300	3	3	\$
32	1	1	35	1	0	340	1140	300	3	3	\$
32	1	1	36	1	0	313	1013	300	3	3	\$
32	1	1	37	1	0	359	1059	300	3	3	\$
32	1	1	38	1	0	315	1015	300	3	3	\$
32	1	1	39	1	0	322	1122	300	3	3	\$
32	1	1	40	1	0	321	1121	300	3	3	\$
32	1	1	41	1	0	323	1123	300	3	3	\$
32	1	1	42	1	0	319	1019	300	3	3	\$
32	1	1	43	1	0	387	1087	300	3	3	\$
32	1	1	44	1	0	311	1111	300	3	3	\$
32	1	1	45	1	0	402	1102	300	4	4	\$
32	1	1	46	1	0	403	0103	300	4	4	\$
32	1	1	47	1	0	440	1140	300	4	4	\$
32	1	1	48	1	0	413	1013	300	4	4	\$
32	1	1	49	1	0	459	1059	300	4	4	\$
32	1	1	50	1	0	415	1015	300	4	4	\$
32	1	1	51	1	0	422	1122	300	4	4	\$
32	1	1	52	1	0	421	1121	300	4	4	\$
32	1	1	53	1	0	423	1123	300	4	4	\$
32	1	1	54	1	0	419	1019	300	4	4	\$
32	1	1	55	1	0	487	1087	300	4	4	\$
32	1	1	56	1	0	411	1111	300	4	4	\$
32	1	1	57	1	0	540	1140	300	5	5	\$
32	1	1	58	1	0	515	1015	300	5	5	\$
32	1	1	59	1	0	522	1122	300	5	5	\$
32	1	1	60	1	0	521	1121	300	5	5	\$
32	1	1	61	1	0	523	1123	300	5	5	\$
32	1	1	62	1	0	519	1019	300	5	5	\$
32	1	1	63	1	0	587	1087	300	5	5	\$
32	1	1	64	1	0	511	1111	300	5	5	\$
32	1	1	65	1	0	002	1102	300	5	1	\$
32	1	1	66	1	0	003	0103	300	5	1	\$
32	1	1	67	1	0	004	1104	300	5	1	\$
32	1	1	68	1	0	005	1105	300	5	1	\$
32	1	1	69	1	0	035	1035	300	5	1	\$
32	1	1	70	1	0	012	1112	300	5	1	\$
32	1	1	71	1	0	009	1009	300	5	1	\$
999	1	1	1	1	0						

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GENERAL DATA

NUMBER OF COMPOSITIONS	5	
NUMBER OF LETHARGY GROUPS	29	
NUMBER OF REGIONS IN X-DIRECTION	5	CYLINDRICAL
NUMBER OF REGIONS IN Y-DIRECTION	1	SLAB
MUG FILE NAME	ZPPR2	
NUMBER OF GROUPS	29	
DOWNSCATTER TO GROUP	29	
MAXIMUM DOWNSCATTER	15	
NUMBER OF MATERIALS	71	
CHI VALUES FROM COMPOSITION	1	
USING FLUX SET	1	


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X X XXXX X X XX XX X X X X X X X
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X-DIRECTION CYLINDRICAL GEOMETRY 5 REGIONS 90 INTERVALS

	REGION	INTERVALS	BOUNDARIES (CM)		REGION WIDTH	MESH WIDTH
	1	1- 40	0,	6,4400E 01	6,4400E 01	1,6100E 00
VOLUME	8,1433E 00	2,4430E 01	4,0717E 01	5,7003E 01	7,3290E 01	8,9577E 01 1,0586E 02 1,2215E 02
	1,3844E 02	1,5472E 02	1,7101E 02	1,8730E 02	2,0358E 02	2,1987E 02 2,3616E 02 2,5244E 02
	2,6873E 02	2,8502E 02	3,0130E 02	3,1759E 02	3,3388E 02	3,5016E 02 3,6645E 02 3,8274E 02
	3,9902E 02	4,1531E 02	4,3160E 02	4,4788E 02	4,6417E 02	4,8046E 02 4,9674E 02 5,1303E 02
	5,2932E 02	5,4560E 02	5,6189E 02	5,7818E 02	5,9446E 02	6,1075E 02 6,2704E 02 6,4332E 02

	REGION	INTERVALS	BOUNDARIES (CM)		REGION WIDTH	MESH WIDTH
	2	41- 60	6,4400E 01	9,1070E 01	2,6670E 01	1,3335E 00
VOLUME	5,4517E 02	5,5634E 02	5,6752E 02	5,7869E 02	5,8986E 02	6,0103E 02 6,1221E 02 6,2338E 02
	6,3455E 02	6,4573E 02	6,5690E 02	6,6807E 02	6,7924E 02	6,9042E 02 7,0159E 02 7,1276E 02
	7,2394E 02	7,3511E 02	7,4628E 02	7,5746E 02		

	REGION	INTERVALS	BOUNDARIES (CM)		REGION WIDTH	MESH WIDTH
	3	61- 75	9,1070E 01	1,0981E 02	1,8740E 01	1,2493E 00
VOLUME	7,1978E 02	7,2959E 02	7,3940E 02	7,4921E 02	7,5901E 02	7,6882E 02 7,7863E 02 7,8843E 02
	7,9824E 02	8,0805E 02	8,1785E 02	8,2766E 02	8,3747E 02	8,4728E 02 8,5708E 02

	REGION	INTERVALS	BOUNDARIES (CM)		REGION WIDTH	MESH WIDTH
	4	76- 85	1,0981E 02	1,2887E 02	1,9060E 01	1,9060E 00
VOLUME	1,3265E 03	1,3493E 03	1,3721E 03	1,3949E 03	1,4178E 03	1,4406E 03 1,4634E 03 1,4863E 03
	1,5091E 03	1,5319E 03				

	REGION	INTERVALS	BOUNDARIES (CM)		REGION WIDTH	MESH WIDTH
	5	86- 90	1,2887E 02	1,4058E 02	1,1710E 01	2,3420E 00
VOLUME	1,9136E 03	1,9480E 03	1,9825E 03	2,0170E 03	2,0514E 03	

Y-DIRECTION

SLAB GEOMETRY

1 REGIONS

1 INTERVALS

	REGION	INTERVALS	BOUNDARIES (CM)	REGION WIDTH	MESH WIDTH
	1	1	0,	1.0000E 00	1.0000E 00
VOLUME	1.0000E 00				

FLUX SOLUTION 1 1-D, X DIRECTION CYLINDRICAL GEOMETRY

8 ACCELERATION CYCLES, 5 ITERATIONS PER CYCLE, LIMIT OF 40 ITERATIONS,

FISSION SOURCE CONVERGENCE = $1.0000E-02$ FOR INTERVALS 1 THRU 1

FLUX CONVERGENCE FOR ELASTIC REMOVAL ITERATIONS = $1.0000E-02$

DELTA-K CONVERGENCE = $1.0000E-03$

LEAKAGE IN X-DIRECTION = $2.5000E-01$ FOR CYCLES 1 THRU 8
 $2.5000E-01$ FOR CYCLES 1 THRU 8

RATIO OF 2ND. MODE BUCKLING TO 1ST, = 3.2960

BOUNDARY CONDITION SET 1 IS USED AT THE LEFT

BOUNDARY CONDITION SET 2 IS USED AT THE RIGHT

REGION	INTERVALS	COMPO- SITION	FLUX SET GENERATED
--------	-----------	------------------	-----------------------

1	1- 40	1	1
2	41- 60	2	2
3	61- 75	3	3
4	76- 85	4	4
5	86- 90	5	5

VII-8

CEAF-13740

COMPOSITION 1

MUG MATERIAL	GMUG MATERIAL	DENSITY	DEG, F	REF, COMP,	FLUX SET FOR SIG-ER CORRECTION
104	1104	8.4330E-04	300.0	1	1
105	1105	1.1230E-04	300.0	1	1
106	1106	1.8200E-05	300.0	1	1
155	1055	1.8000E-06	300.0	1	1
102	1102	1.2300E-05	300.0	1	1
103	103	5.5550E-03	300.0	1	1
140	1140	3.0000E-05	300.0	1	1
113	1013	1.3120E-02	300.0	1	1
159	1059	8.7960E-03	300.0	1	1
115	1015	1.4000E-04	300.0	1	1
122	1122	1.2580E-02	300.0	1	1
121	1121	2.7020E-03	300.0	1	1
123	1123	1.2210E-03	300.0	1	1
119	1019	2.0900E-04	300.0	1	1
187	1087	1.9000E-05	300.0	1	1
111	1111	2.3100E-04	300.0	1	1

COMPOSITION 2

MUG MATERIAL	GMUG MATERIAL	DENSITY	DEG, F	REF, COMP,	FLUX SET FOR SIG-ER CORRECTION
204	1104	1.2740E-03	300.0	2	2
205	1105	1.6960E-04	300.0	2	2
206	1106	2.7400E-05	300.0	2	2
255	1055	2.8000E-06	300.0	2	2
202	1102	1.1500E-05	300.0	2	2
203	103	5.1980E-03	300.0	2	2
240	1140	2.3000E-05	300.0	2	2
213	1013	1.1760E-02	300.0	2	2
259	1059	8.2640E-03	300.0	2	2
215	1015	1.2200E-04	300.0	2	2
222	1122	1.3850E-02	300.0	2	2
221	1121	2.5230E-03	300.0	2	2
223	1123	1.1600E-03	300.0	2	2
219	1019	2.0200E-04	300.0	2	2
287	1087	2.0000E-05	300.0	2	2
211	1111	3.4100E-04	300.0	2	2

COMPOSITION 3

MUG MATERIAL	GMUG MATERIAL	DENSITY	DEG.F	REF, COMP;	FLUX SET FOR SIG-ER CORRECTION
302	1102	2,4000E-05	300,0	3	3
303	103	1,1080E-02	300,0	3	3
340	1140	1,0130E-03	300,0	3	3
313	1013	2,0130E-02	300,0	3	3
359	1059	6,3980E-03	300,0	3	3
315	1015	9,6000E-05	300,0	3	3
322	1122	6,9230E-03	300,0	3	3
321	1121	1,9910E-03	300,0	3	3
323	1123	8,9800E-04	300,0	3	3
319	1019	1,5700E-04	300,0	3	3
387	1087	1,7000E-05	300,0	3	3
311	1111	1,4000E-05	300,0	3	3

COMPOSITION 4

MUG MATERIAL	GMUG MATERIAL	DENSITY	DEG.F	REF, COMP;	FLUX SET FOR SIG-ER CORRECTION
402	1102	2,4000E-05	300,0	4	4
403	103	1,1080E-02	300,0	4	4
440	1140	1,0130E-03	300,0	4	4
413	1013	2,0130E-02	300,0	4	4
459	1059	5,9630E-03	300,0	4	4
415	1015	1,0500E-04	300,0	4	4
422	1122	7,5410E-03	300,0	4	4
421	1121	2,1720E-03	300,0	4	4
423	1123	9,8700E-04	300,0	4	4
419	1019	1,7400E-04	300,0	4	4
487	1087	1,8000E-05	300,0	4	4
411	1111	1,5000E-05	300,0	4	4

COMPOSITION

MUG MATERIAL	GMUG MATERIAL	DENSITY	DEG. F	REF, COMP.	FLUX SET FOR SIG-ER CORRECTION
540	1140	5,5800E-04	300,0	5	5
515	1015	9,1000E-05	300,0	5	5
522	1122	7,5161E-02	300,0	5	5
521	1121	1,2050E-03	300,0	5	5
523	1123	5,1300E-04	300,0	5	5
519	1019	5,9800E-04	300,0	5	5
587	1087	1,3000E-05	300,0	5	5
511	1111	1,2000E-05	300,0	5	5
35	1035	1,0000E-12	300,0	5	1
12	1112	1,0000E-12	300,0	5	1
2	1102	1,0000E-12	300,0	5	1
3	1103	1,0000E-12	300,0	5	1
4	1104	1,0000E-12	300,0	5	1
5	1105	1,0000E-12	300,0	5	1
9	1009	1,0000E-12	300,0	5	1

FLUX SOLUTION 1 HISTORY

CYCLE	ITERATION	REACTIVITY	(CHANGE)	MAX, FISSION SOURCE CHANGE	AT
1	1	0.97336	9.73363E-01	0.	0
1	2	0.99042	1.70571E-02	0.	0
1	3	0.98831	2.11442E-03	0.	0
1	4	0.99179	3.48228E-03	0.	0
1	5	0.99140	3.91901E-04	9.93761E-03	1

FISSION SOURCE CONVERGED

The flux solution history for 11 iterations was deleted to conserve space.

FLUX SOLUTION 1 HISTORY

CYCLE	ITERATION	REACTIVITY	(CHANGE)	MAX, FISSION SOURCE CHANGE	AT
1	1	0.98486	9.8486E-01	0.	0
1	2	0.98484	2.29031E-05	1.31942E-05	1

FISSION SOURCE CONVERGED

REGION FLUX	MAX, CHANGE	REGION	GROUP	GROUPS NOT CONVERGED
-------------	-------------	--------	-------	-------------------------

1.1093E-03	1	14	0
2.9806E-04	2	5	0
4.3329E-03	3	14	0
8.1739E-03	4	14	0
8.4316E-03	5	12	0

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FLUX SET NUMBER 1

1	1.08416E 04	2	4.46797E 04	3	1.08850E 03	4	1.52920E 03	5	1.95774E 03
6	3.55345E 03	7	3.25440E 03	8	4.57553E 03	9	4.29689E 03	10	3.85576E 03
11	2.73152E 05	12	2.08916E 05	13	2.34974E 05	14	1.54105E 05	15	9.39973E 04
16	4.64492E 04	17	1.30381E 04	18	3.87195E 04	19	3.93323E 04	20	2.06639E 04
21	8.70823E 03	22	4.75971E 03	23	1.73621E 03	24	5.68693E 02	25	1.26582E 02
26	4.27274E 01	27	1.17188E 01	28	1.71845E 00	29	1.77140E -02

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FLUX SET NUMBER 2

1	8.60985E 03	2	3.96063E 04	3	8.43207E 04	4	1.17512E 03	5	1.49401E 03
6	2.57418E 05	7	2.41873E 05	8	3.22450E 05	9	2.92304E 05	10	2.51525E 05
11	1.80172E 05	12	1.85253E 05	13	1.40470E 05	14	9.08884E 04	15	5.43466E 04
16	2.61571E 04	17	8.01663E 03	18	3.28556E 04	19	2.09890E 04	20	1.06916E 04
21	4.38469E 03	22	2.36588E 03	23	8.32616E 02	24	2.67692E 02	25	6.59452E 01
26	3.12712E 01	27	8.68543E 00	28	2.26209E 00	29	3.99717E 02

1	1.58331E	03	2	6.38962E	03	3	1.59352E	04	4	2.29875E	04	5	3.48200E	04
6	8.61387E	04	7	9.86335E	04	8	1.17682E	05	9	1.07835E	05	10	9.90024E	04
11	9.22636E	04	12	5.54765E	04	13	4.28849E	04	14	3.72314E	04	15	2.46714E	04
16	1.87810E	04	17	1.34756E	04	18	1.82230E	04	19	1.56170E	04	20	1.03696E	04
21	5.71126E	03	22	3.79251E	03	23	1.72742E	03	24	6.87028E	02	25	4.29866E	02
26	1.70977E	02	27	5.36466E	01	28	1.55430E	01	29	2.91682E	00			

615T-13/40

1	2,11503E	02	2	8,18004E	02	3	2,127698E	03	4	3,45226E	03	5	5,36386E	03
6	2,34972E	04	7	3,23884E	04	8	4,100460E	04	9	3,76609E	04	10	3,52487E	04
11	3,96923E	04	12	2,60736E	04	13	1,67281E	04	14	1,55398E	04	15	1,05569E	04
16	8,70721E	03	17	6,99745E	03	18	9,10531E	03	19	8,55998E	03	20	7,48634E	03
21	4,06785E	03	22	3,93684E	03	23	2,27506E	03	24	1,06078E	03	25	7,32089E	02
26	3,32702E	02	27	1,19207E	02	28	3,04657E	01	29	5,30464E	00			

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[illegible]

MUG FILE EDIT,

TAPE ID "TDMUG2"
FILE ID "ZPPR2 "

CHI VALUES,

3.219635E-02	1.210760E-01	2.105033E-01	2.231693E-01	1.733207E-01	1.109715E-01	6.309721E-02	3.336379E-02
1.687794E-02	8.311331E-03	3.944292E-03	1.661557E-03	7.720968E-04	3.762472E-04	1.783271E-04	8.440819E-05
3.992103E-05	1.887153E-05	8.918335E-06	4.213884E-06	1.990830E-06	9.404964E-07	4.442862E-07	2.090736E-07
9.913950E-08	4.683081E-08	3.749918E-08	3.952414E-09	4.155820E-10			

DELU VALUES,

5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01
5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01
5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01	5.000000E-01
5.000000E-01	5.000000E-01	1.500000E 00	1.500000E 00	1.500000E 00			

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INELASTIC SCATTERING MATRIX

MATERIAL 104

GROUP

1	3.62655E-02 1.10389E-02	7.86894E-02 4.33577E-03	2.08071E-01 1.65973E-03	2.05082E-01 6.25495E-04	2.10722E-01 2.33201E-04	1.24734E-01 8.66666E-05	6.13507E-02 5.07907E-05	2.69419E-02
2	8.07740E-02 9.49246E-03	2.26983E-01 3.66777E-03	3.78008E-01 1.39011E-03	3.27215E-01 5.20725E-04	2.55362E-01 1.93677E-04	1.23784E-01 7.17257E-05	5.66438E-02 4.19624E-05	2.38001E-02
3	2.56086E-01 5.00202E-03	3.23807E-01 1.90712E-03	3.67702E-01 7.16980E-04	2.71716E-01 2.67258E-04	1.23390E-01 9.91069E-05	7.33044E-02 3.66365E-05	3.16271E-02 2.14045E-05	1.28193E-02
4	4.45702E-01 1.73555E-03	2.75685E-01 6.54079E-04	2.20045E-01 2.44174E-04	1.30297E-01 9.06287E-03	6.41229E-02 3.35207E-05	2.81664E-02 1.23720E-03	1.15420E-02 7.22017E-06	4.53367E-03
5	4.92936E-01 3.49073E-04	2.69117E-01 1.37021E-04	8.83883E-02 4.84638E-03	5.23618E-02 1.79334E-03	2.07223E-02 6.62077E-06	6.74015E-03 2.44089E-06	2.58258E-03 1.42366E-06	9.60996E-04
6	3.73068E-01 4.63513E-05	2.12912E-01 3.53808E-05	7.74973E-02 0.	3.50108E-02 0.	1.18520E-02 0.	5.12700E-03 0.	1.20552E-03 0.	4.48441E-04
7	2.36535E-01 5.31047E-06	5.84506E-02 1.07232E-06	3.51967E-02 0.	1.78012E-02 0.	8.93762E-03 0.	4.30888E-03 0.	5.26240E-04 0.	2.93471E-04
8	2.48062E-01 0.	3.19528E-03 0.	3.09314E-04 4.39670E-08	1.04107E-04 0.	2.28034E-05 0.	9.96284E-04 0.	5.89151E-04 0.	1.92169E-04
9	2.07272E-01 0.	5.31749E-02 0.	2.97389E-03 0.	4.17254E-06 0.	5.42831E-06 0.	2.89762E-06 0.	0. 0.	5.25837E-07
10	1.39038E-01 0.	3.84830E-02 0.	2.05645E-02 0.	6.28065E-03 0.	5.49384E-04 0.	9.21847E-05 0.	5.87701E-05 0.	2.82677E-05
11	1.53763E-01 1.70746E-05	0. 0.	9.68438E-04 0.	2.14296E-03 0.	1.12467E-03 0.	1.73508E-04 0.	9.46396E-05 0.	0.
12	2.00205E-01 0.	0. 0.	0. 0.	0. 0.	0. 0.	0. 0.	0. 0.	0.
13	1.04100E-01 0.	2.46175E-02 0.	0. 0.	0. 0.	0. 0.	0. 0.	0. 0.	0.
14	0. 0.	1.30085E-02 0.	1.57871E-02 0.	6.12192E-03 0.	2.89234E-03 0.	4.52034E-04 0.	0. 0.	0.
15	0. 0.	0. 0.	0. 0.	0. 0.	7.50749E-04 0.	5.19263E-04 0.	1.14835E-05 0.	0.

16 - 28 ARE ALL 0.0

MATERIAL 104

GROUP

TRANSPORT

FISSION

CAPTURE

ELASTIC

INELASTIC

NU

1	3.84972E 00	2.08825E 00	1.25536E-03	1.19220E-02	9.49794E-01	3.98024E 00
2	4.31092E 00	1.70853E 00	1.78897E-03	1.13992E-02	1.49765E 00	3.53485E 00
3	4.89910E 00	1.94548E 00	3.98179E-03	1.04907E-02	1.49850E 00	3.26637E 00
			1.03736E-02	2.03465E-02	1.18287E 00	3.11123E 00

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5	5,18425E 00	1,75180E 00	2,46276E-02	4,75265E-02	9,34372E-01	3,01766E 00
6	5,18169E 00	1,63022E 00	7,50048E-02	5,07489E-02	7,15184E-01	2,96368E 00
7	6,86517E 00	1,55539E 00	1,40755E-01	9,99006E-02	3,62056E-01	2,93102E 00
8	8,21056E 00	1,49362E 00	1,95975E-01	1,03616E-01	2,53469E-01	2,91091E 00
9	9,50884E 00	1,54082E 00	2,30444E-01	1,22624E-01	2,63434E-01	2,89870E 00
10	1,07731E 01	1,63244E 00	2,69863E-01	1,27450E-01	2,05495E-01	2,89135E 00
11	1,20062E 01	1,70216E 00	3,63155E-01	1,47266E-01	1,58284E-01	2,88689E 00
12	1,30131E 01	1,74272E 00	5,57594E-01	1,88970E-01	2,00205E-01	2,88418E 00
13	1,34659E 01	1,79460E 00	7,77890E-01	1,54771E-01	1,28717E-01	2,88224E 00
14	1,44589E 01	1,94632E 00	1,07107E 00	1,60168E-01	3,82619E-02	2,88136E 00
15	1,58750E 01	2,20019E 00	1,59130E 00	1,56686E-01	1,28150E-03	2,88083E 00
16	1,72717E 01	2,59086E 00	2,21897E 00	1,39387E-01	0,	2,88050E 00
17	1,92037E 01	3,16842E 00	3,11526E 00	5,88694E-01	0,	2,88031E 00
18	1,98745E 01	4,23025E 00	3,46646E 00	1,88630E-01	0,	2,88018E 00
19	2,26735E 01	5,75343E 00	4,24729E 00	1,88870E-01	0,	2,88011E 00
20	2,74722E 01	8,61191E 00	6,29092E 00	1,90340E-01	0,	2,88007E 00
21	2,90206E 01	9,02649E 00	7,43810E 00	1,99741E-01	0,	2,88004E 00
22	3,12166E 01	1,52800E 01	6,74880E 00	1,58156E-01	0,	2,88003E 00
23	3,60396E 01	1,78770E 01	1,11496E 01	1,70632E-01	0,	2,88002E 00
24	4,07172E 01	2,88984E 01	8,32624E 00	1,78831E-01	0,	2,88001E 00
25	5,31577E 01	3,28981E 01	2,82805E 01	1,86899E-01	0,	2,88001E 00
26	2,48644E 01	9,93122E 00	1,03628E 01	1,31740E-01	0,	2,88000E 00
27	5,45700E 01	4,31644E 01	2,90061E 01	3,64534E-02	0,	2,88000E 00
28	3,27370E 00	3,78652E 00	8,50250E-01	3,03606E-02	0,	2,88000E 00
29	2,12323E 02	2,87977E 02	1,76784E 02	0,	0,	2,88000E 00

The edits of the other material cross section sets have been
deleted to conserve space.

SELF SHIELDED CROSS SECTIONS*

MUG MATERIAL 35

1	1.0000E 00	2	1.0000E 00	3	1.0000E 00	4	1.0000E 00	5	1.0000E 00
6	1.0000E 00	7	1.0000E 00	8	1.0000E 00	9	1.0000E 00	10	1.0000E 00
11	1.0000E 00	12	1.0000E 00	13	1.0000E 00	14	1.0000E 00	15	1.0000E 00
16	1.0000E 00	17	1.0000E 00	18	1.0000E 00	19	1.0000E 00	20	1.0000E 00
21	1.0000E 00	22	1.0000E 00	23	1.0000E 00	24	1.0000E 00	25	1.0000E 00
26	1.0000E 00	27	1.0000E 00	28	1.0000E 00	29	1.0000E 00		

MUG MATERIAL 102

1	1.0000E 00	2	1.0000E 00	3	1.0000E 00	4	1.0000E 00	5	1.0000E 00
6	1.0000E 00	7	1.0000E 00	8	1.0000E 00	9	1.0000E 00	10	1.0000E 00
11	1.0000E 00	12	2.9348E 04	13	2.1647E 04	14	2.3494E 04	15	3.6115E 04
16	4.3653E 04	17	8.9831E 04	18	2.720E 04	19	3.0096E 04	20	2.7943E 04
21	3.9288E 04	22	3.0292E 04	23	3.1924E 04	24	3.0960E 04	25	3.4594E 04
26	2.8651E 04	27	3.5865E 04	28	2.8541E 04	29	3.1781E 04		

MUG MATERIAL 103

1	1.0000E 00	2	1.0000E 00	3	1.0000E 00	4	1.0000E 00	5	1.0000E 00
6	1.0000E 00	7	1.0000E 00	8	1.0000E 00	9	1.0000E 00	10	1.0000E 00
11	3.5459E 01	12	5.2522E 01	13	3.4755E 01	14	4.2859E 01	15	6.5794E 01
16	8.1552E 01	17	1.8189E 02	18	5.8189E 01	19	3.2951E 01	20	4.9085E 01
21	7.3985E 01	22	5.2125E 01	23	2.4913E 01	24	5.7054E 01	25	6.3130E 01
26	5.2752E 01	27	6.3856E 01	28	2.4169E 01	29	1.0000E 00		

MUG MATERIAL 104

1	1.0000E 00	2	1.0000E 00	3	1.0000E 00	4	1.0000E 00	5	1.0000E 00
6	1.0000E 00	7	1.0000E 00	8	1.0000E 00	9	1.0000E 00	10	1.0000E 00
11	1.0000E 00	12	4.1762E 02	13	3.0227E 02	14	4.3752E 02	15	5.1101E 02
16	6.1952E 02	17	1.2911E 03	18	4.5706E 02	19	4.1542E 02	20	3.7789E 02
21	5.4152E 02	22	4.0596E 02	23	4.2042E 02	24	3.9602E 02	25	4.3093E 02
26	3.8310E 02	27	4.2338E 02	28	4.0922E 02	29	6.0830E 02		

MUG MATERIAL 105

1	1.0000E 00	2	1.0000E 00	3	1.0000E 00	4	1.0000E 00	5	1.0000E 00
6	1.0000E 00	7	1.0000E 00	8	1.0000E 00	9	1.0000E 00	10	1.0000E 00
11	1.0000E 00	12	3.2235E 03	13	2.3578E 03	14	2.7789E 03	15	3.9410E 03
16	4.7662E 03	17	9.8219E 03	18	3.3642E 03	19	3.2734E 03	20	3.0444E 03
21	4.2743E 03	22	3.3010E 03	23	3.4451E 03	24	3.2913E 03	25	3.6901E 03
26	3.1424E 03	27	3.9166E 03	28	2.9102E 03	29	7.3966E 03		

MUG MATERIAL 106

1	1.0000E 00	2	1.0000E 00	3	1.0000E 00	4	1.0000E 00	5	1.0000E 00
6	1.0000E 00	7	1.0000E 00	8	1.0000E 00	9	1.0000E 00	10	1.0000E 00
11	1.0000E 00	12	1.0000E 00	13	1.0000E 00	14	1.0000E 00	15	1.0000E 00
16	1.0000E 00	17	1.0000E 00	18	1.0000E 00	19	1.0000E 00	20	1.0000E 00
21	1.0000E 00	22	1.0000E 00	23	1.0000E 00	24	1.0000E 00	25	1.0000E 00
26	1.0000E 00	27	1.0000E 00	28	1.0000E 00	29	1.0000E 00		

*A value of 1.0000E00 for the self-shielded cross section indicates the material cross sections do not self-shield in that group.

The edits of the other material self-shielding parameters have been deleted to conserve space.

REFERENCES

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3. B. A. Hutchins, C. L. Cowan, M. D. Kelley and J. E. Turner, "ENDRUN-II - A Computer Code to Generate A Generalized Multigroup Data File from ENDF/B", GEAP-13704, March 1971.
4. G. I. Bell, "A Single Treatment for Effective Resonance Absorption Cross Sections in Dense Lattices", Nuc. Sci. and Eng. 2 Pg. 138, (1959).
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APPENDIX A

GMUG AND MUG FILE DESCRIPTIONS

1. GMUG FILE

A GMUG file consists of generalized multigroup nuclear constants for one or more ENDF/B materials. GMUG materials are described by several data classes, each data class consisting of a data type. The GMUG file described here can have up to seven data classes for each material.*

Each data class on the GMUG is identified by a six-digit word determined by the ENDRUN⁽³⁾ problem generating the data class. Normally the first four digits will be the ENDF/B material number. The last two digits indicate the data type.

A. GMUG File Format and Contents

The GMUG file is blocked at 320 words.** The first block contains information about the energy group structure of the file, consequently this information must be applicable to all materials on the file.

BLOCK 1 File Data

<u>Word(s)</u>	<u>Contents</u>
1-55	IDENT(I) - Tape Label
56	NCL - Number of data classes
57	ITOT - Number of lethargy groups
58-99	Not used

*Presently only seven data classes have been defined. The GMUG file can have any number of data classes to describe a material.

**A block is a physical record on the GMUG tape. Two blocks, 640 words, make up a logical record.

WORD(S)Contents

100

SLETH - Upper lethargy of first
lethargy group.

NOTE: The GMUG file group structure
is given in increasing lethargy
i.e., group 1 has the highest
energy.

101-200

DELU(1-ITOT) Lethargy width of coarse groups

201-300

EL(1-ITOT) Lower energy values of all coarse
groups

BLOCKS 2-20 File DirectoryWord(s)Contents

1

NDICT (1,N) - Class word, a 12-digit
word (in octal) where digits
1-5 identify the starting block for
a data class.
6-7 identifies the source of the
data class when the GMUG file
was created.*
8-12 are a count of the number of
blocks in the data class

2

NDICT (2,N) - 6-digit data class
identification where the first
four are the GMUG material number
and the last two specify the data type.

NDICT (1,N), NDICT (2,N) are repeated in
pairs until all data classes have
been defined in the directory.

*This identifier is the file code number, used in PUNT, of the tape
originally containing the data class. (See Appendix C).

BLOCKS 21 + GMUG DATA Classes

The data class consists of as many blocks as are necessary to contain the class information. The class identification, same as NDICT (2,N), is the first and only word in the beginning block of a data class.

B. Description of Data Classes

DATA SET 1 - General File Data

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-50	IDENT	BCD identification of material and pertinent comments (hollerith)
51	MATT	GMUG material number (integer)
52	AWR	Atomic Weight (Neutron scale) (floating point)
53	LFI	Fission indicator (1=yes, 0=no) (integer)
54	ITOT	Number of lethargy groups (must equal work 57 of BLOCK 1) (Integer)
55	EA	Cutoff energy for fission neutron spectra (floating point)
56-99		Not used at present
100	NSGO	Number of σ_0 's for self-shielding (integer)
101	NTT	Number of temperatures for self-shielding (integer)
102-106	SCO(1-NSGO)	σ_0 values for f-factors (floating point)
107-111	XX(1-NSGO)	Log values of σ_0 's for f-factor interpolation (floating point)
112	LFT	Lowest numbered lethargy group having self-shielding f-factors (highest energy) (integer)
113	LGT	Highest numbered lethargy group having self-shielding f-factors (lowest energy) (integer).

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
114-116	TT(1-NTT)	Temperatures for self-shielding resonance calculation (floating point)
117-125		Not used at present
126	LINELS	Inelastic matrix indicator (1=yes, 0=no) (integer)
127	ILINM	Highest numbered lethargy group having an inelastic matrix (integer)
128	NDSC	Maximum number of inelastic downscatter groups (integer)
129	LGP	Highest numbered lethargy group having an inelastic source term (integer)
130-150		Not used at present
151	LELASM	Elastic matrix indicator (1=yes, 0=no) (integer)
152	IMINEL	Lowest numbered lethargy group having an elastic matrix (integer)
153	IMAXEL	Highest numbered lethargy group having an elastic matrix (integer)
154	KMAXEL	Maximum number of elastic down- scattering groups (integer)
155-175		Not used at present
176	LN2N	(n,2n) matrix indicator (1=yes, 0=no) (integer)
177	ILNNM	Highest numbered lethargy group having an (n,2n) matrix (integer)
178	NDSCN	Maximum number of (n,2n) down- scatter groups (integer)
179	LGPN2N	Highest numbered lethargy group having an (n,2n) source term (integer)
180-320		Not used at present

DATA SET 2 - Infinitely Dilute Coarse Group Averages

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-N	STXI(ICT,I)	<p>Infinitely dilute coarse group average value of reaction number ICT for group I ICT varies from 1 to 15 I varies from 1 to ITOT N = 15*ITOT = length of array</p>

Output reaction indices and their meanings are given below:

<u>ICT</u>	<u>Reaction Meaning</u>
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	Average lethargy loss per collision by elastic scattering
8	Average cosine of elastic scattering angle
9	(n,2n)
10	(n,3n)
11	Average number of neutrons released per fission
12	Elastic removal
13	Fraction of fission neutrons emitted in this energy group
14	LGI = lethargy gain indicator

$$= 1 \quad \ln \frac{1}{\alpha} \leq \frac{\Delta u_{I+1}}{2}$$

$$= 2 \quad \frac{\Delta u_{I+1}}{2} < \ln \frac{1}{\alpha} \leq \Delta u_{I+1}$$

$$= 3 \quad \ln \frac{1}{\alpha} > \Delta u_{I+1}$$

<u>ICT</u>	<u>Reaction Meaning</u>
15	Blank at present

DATA SET 3 - f_o Self-Shielding Factors for Interpolation with Total Cross Section to Obtain σ_o Values

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-N	FFACO(K,L,I)	<p>This array of self-shielding factors is used by TDOWN to determine the proper σ_o for each material of a given core composition. The f_o, determined by interpolating the data of this array, is used to factor the total cross section in the iteration procedure to calculate σ_o.</p> <p>I (coarse group) varies from LFT to LGT; K(σ_o) varies from 1 to NSGO; L (Temp.) varies from 1 to NTT, N = (LGT-LFT+1)*NSGO</p> <p>*NTT = array length</p>

DATA SET 4 - Self-Shielding Factors for Basic Cross Section

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-N	STX(K,L,ICT,I)	<p>Self-shielding factors are included for total, elastic scattering, capture, and fission (if given) according to ICT indices listed in Data Set 2. Several σ_o's and temperatures are given to allow interpolation</p> <p>ICT varies from 1 to 3+LFI (fission indicator)</p> <p>I(coarse group) varies from LFT to LGT</p> <p>K(σ_o) varies from 1 to NSGO</p> <p>L (Temp) varies from 1 to NTT</p> <p>N = (3+LFI)*(LGT-LFT+1)*NSGO*NTT= array length</p>

DATA SET 5 - Elastic Matrix

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-N	SNIN(I,K)	<p>The elastic matrix terms are given as fractions of $\sigma_{er,I}$ with the in-group scattering term set to zero. The matrix is normalized so that the sum of the terms over $M>I$, for each I, is equal to 1.</p> <p>I (source group) varies from 1 to minimum of IMINEL or 70.</p> <p>M (downscattering group) varies from I to $(KMAXEL+I)$</p> <p>$N = \min(ITOT,70)(KMAXEL+1) = \text{array length}$</p>

DATA SET 6 - Inelastic Matrix

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-N	SXIN(I,K)	<p>The inelastic matrix terms are $\sigma_{in}(I \rightarrow M)$ where in-group scattering is included. The matrix is normalized such that</p>

$$\sum_m \sigma_{in}(I \rightarrow M) = \sigma_{in,I}$$

If only one combined matrix is desired, it is put in this Data Set, and normalized such that

$$\sum_M \sigma(I \rightarrow M) = \sigma_{es,I} + \sigma_{in,I} + 2\sigma_{n,2n,I} + 3\sigma_{n,3n,I}$$

I (source group) varies first from 1 to ILINM

M (downscattering group) varies second from I to $(NDSC+I)$

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
		$N = \text{ILINM}(\text{NDSC}+1) = \text{array length}$

DATA SET 7 - Combined (n,2n)/(n,3n) Matrix

<u>Word</u>	<u>Notation</u>	<u>Definition</u>
1-N	$\text{SX2N}(\text{I},\text{K})$	The (n,2n) and (n,3n) matrices are combined and include in-group scattering as in Data Set 6. The matrix is normalized so that

$$\sum_M \sigma_{n,2n}^{(\text{I} \rightarrow \text{M})} = 2\sigma_{n,2n,\text{I}} + 3\sigma_{n,3n,\text{I}}$$

I (source group) varies first from 1 to ILNNM

M(downscattering group) varies second from I to (NDSC+I)

$N = \text{ILNNM} (\text{NDSC}+1) = \text{array length}$

A sample listing of a GMUG material is given on the following pages. The sample includes all data sets except Data Set 5 the elastic matrix.

The information for data classes 1, 2, and 3 is easily identified by referring to the data set descriptions. Data class set 4 consists of f-factors for total, elastic scattering, capture and fission in order. Data class set 6 lists the inelastic scattering terms for each group (reading across) beginning with $\text{I} \rightarrow \text{I}$, $\text{I} \rightarrow \text{I}+1$ $\text{I} \rightarrow \text{I}+\text{NDSC}$. Data class set 7, the n-2n matrix terms, lists the terms, $\text{I} \rightarrow \text{I}$, $\text{I} \rightarrow \text{I}+1$, $\text{I} \rightarrow \text{I}+\text{NDSC}$ in columns (read downward).

DATA SET 1 1104

PU239

MATT 1104	LFI 1	ITOT 29	NSGO 4	NTT 1	LFT 12	LGT 29	LINEL5 1	ILINM 16	NDSC 15	LGP 0
LELASH 0	IMINEL 0	IMAXEL 0	KMAXEL 0	LN2N 1	ILNNM 3	NDSC 15	LGPN2N 0			

AWR 236.999 E(A) 0.250000E 07

XX	1.00000	2.00000	3.00000	4.00000	0.
SGO	10.0000	100.000	1000.00	10000.0	0.
TT	300	0	0		

A-9

GEAR-13740

DATA SET 2 1104

	TOTAL	ELASTIC	CAPTURE	FISSION	TOTAL	INELASTIC	XI
1	6.687	3.156	0.1307E-02	2.040	0.	1.410	0.9131E-03
2	7.810	3.924	0.2624E-02	1.710	0.	2.172	0.1008E-02
3	7.801	3.558	0.5369E-02	1.845	0.	2.393	0.1410E-02
4	7.178	2.852	0.1126E-01	1.938	0.	2.376	0.2244E-02
5	7.241	3.410	0.2388E-01	1.718	0.	2.089	0.3305E-02
6	8.130	4.817	0.5216E-01	1.594	0.	1.667	0.4281E-02
7	9.191	6.342	0.1246	1.517	0.	1.208	0.5317E-02
8	10.21	7.662	0.1842	1.504	0.	0.8553	0.6242E-02
9	11.20	8.820	0.2113	1.499	0.	0.6739	0.6806E-02
10	12.16	9.883	0.2363	1.497	0.	0.5396	0.7238E-02
11	12.96	10.66	0.3175	1.553	0.	0.4335	0.7669E-02
12	13.58	11.08	0.4867	1.638	0.	0.3748	0.8017E-02
13	14.21	11.63	0.6568	1.760	0.	0.1654	0.8244E-02
14	14.83	11.95	0.9691	1.871	0.	0.3826E-01	0.8381E-02
15	16.18	12.56	1.502	2.123	0.	0.1281E-02	0.8415E-02
16	17.50	12.91	2.164	2.430	0.	0.	0.8415E-02
17	19.14	13.14	2.976	3.028	0.	0.	0.8415E-02
18	20.86	13.05	3.630	4.179	0.	0.	0.8415E-02
19	23.81	13.15	4.652	6.004	0.	0.	0.8415E-02
20	29.92	14.32	6.599	8.994	0.	0.	0.8415E-02
21	33.86	14.56	9.075	10.23	0.	0.	0.8415E-02
22	40.29	13.74	8.758	17.79	0.	0.	0.8415E-02
23	52.32	14.44	15.81	22.07	0.	0.	0.8415E-02
24	77.90	16.56	15.57	45.77	0.	0.	0.8415E-02
25	122.1	17.96	57.96	46.13	0.	0.	0.8415E-02
26	40.47	9.541	15.93	15.00	0.	0.	0.8415E-02
27	140.4	11.03	51.12	78.29	0.	0.	0.8415E-02
28	724.4	15.41	115.7	593.3	0.	0.	0.8415E-02
29	1471.	13.00	528.4	930.1	0.	0.	0.8415E-02

GEAP-13740

	MU	N-2N	N-3N	NU	ELS, REMOVAL	CHI	LGI	
1	0.9130	0.8029E-01	0.	3.977	0.1185E-01	0.3248E-01	1.000	0.
2	0.8910	0.2918E-03	0.	3.534	0.1129E-01	0.1218	1.000	0.
3	0.8383	0.	0.	3.268	0.1082E-01	0.2109	1.000	0.
4	0.7364	0.	0.	3.111	0.1280E-01	0.2230	1.000	0.
5	0.6091	0.	0.	3.018	0.2254E-01	0.1728	1.000	0.
6	0.4931	0.	0.	2.964	0.4124E-01	0.1105	1.000	0.
7	0.3701	0.	0.	2.931	0.6744E-01	0.6275E-01	1.000	0.
8	0.2604	0.	0.	2.911	0.9565E-01	0.3316E-01	1.000	0.
9	0.1935	0.	0.	2.899	0.1201	0.1677E-01	1.000	0.
10	0.1423	0.	0.	2.891	0.1431	0.8256E-02	1.000	0.
11	0.9128E-01	0.	0.	2.887	0.1634	0.3999E-02	1.000	0.
12	0.5004E-01	0.	0.	2.884	0.1777	0.1918E-03	1.000	0.
13	0.2308E-01	0.	0.	2.883	0.1917	0.9144E-03	1.000	0.
14	0.6866E-02	0.	0.	2.882	0.2104	0.2059E-03	1.000	0.
15	0.2813E-02	0.	0.	2.881	0.2114	0.9746E-04	1.000	0.
16	0.2813E-02	0.	0.	2.881	0.2173	0.4609E-04	1.000	0.
17	0.2813E-02	0.	0.	2.880	0.2211	0.2179E-04	1.000	0.
18	0.2813E-02	0.	0.	2.880	0.217	0.1030E-04	1.000	0.
19	0.2813E-02	0.	0.	2.880	0.2213	0.4866E-05	1.000	0.
20	0.2813E-02	0.	0.	2.880	0.2411	0.2299E-05	1.000	0.
21	0.2813E-02	0.	0.	2.880	0.2450	0.1086E-05	1.000	0.
22	0.2813E-02	0.	0.	2.880	0.2312	0.5130E-06	1.000	0.
23	0.2813E-02	0.	0.	2.880	0.2430	0.2423E-06	1.000	0.
24	0.2813E-02	0.	0.	2.880	0.2787	0.1145E-06	1.000	0.
25	0.2813E-02	0.	0.	2.880	0.3023	0.5407E-07	1.000	0.
26	0.2813E-02	0.	0.	2.880	0.1606	0.4330E-07	1.000	0.
27	0.2813E-02	0.	0.	2.880	0.6189E-01	0.4564E-08	1.000	0.
28	0.2813E-02	0.	0.	2.880	0.8443E-01	0.4810E-09	1.000	0.
29	0.2813E-02	0.	0.	2.880	0.7294E-01			

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F-FACTORS. DATA SET 3.

12	0.9997514	0.9999291	0.9999960	0.9999993
13	0.9897909	0.9970636	0.9997769	0.9999526
14	0.9805590	0.9938615	0.9991499	0.9999269
15	0.9614002	0.9862076	0.9980163	0.9993984
16	0.9296176	0.9712594	0.9956791	0.9990383
17	0.8918119	0.9509253	0.9928572	0.9992022
18	0.8527775	0.9257675	0.9886950	0.9985955
19	0.7904087	0.8809597	0.9795502	0.9976381
20	0.6891136	0.7980376	0.9555174	0.9945822
21	0.5377751	0.7288787	0.9358855	0.9919987
22	0.5780765	0.7418592	0.9358339	0.9922274
23	0.4563465	0.6306219	0.8818429	0.9835618
24	0.3733058	0.5000646	0.7552615	0.9532238
25	0.2160211	0.3866703	0.7252277	0.9507002
26	0.4030567	0.5639379	0.8438111	0.9776255
27	0.2348219	0.3572181	0.6779814	0.9392063
28	0.0829013	0.1379755	0.3604191	0.7836957
29	0.1516064	0.2039668	0.4459148	0.8396158

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F-FACTORS. DATA SET 4 MATERIAL 1104

12	0.9995573	0.9998693	0.9999758	1.0000000
13	0.9815291	0.9944407	0.9992740	0.9999810
14	0.9692269	0.9877953	0.9984117	0.9995432
15	0.9341014	0.9731051	0.9962688	0.9993581
16	0.8844445	0.9455317	0.9920712	0.9990599
17	0.8286395	0.9092219	0.9862088	0.9985660
18	0.7731762	0.8670768	0.9776710	0.9974733
19	0.6924283	0.7998351	0.9603106	0.9954755
20	0.5711041	0.6898151	0.9166770	0.9894031
21	0.3595601	0.5949537	0.8815561	0.9844236
22	0.4664735	0.6194309	0.8818551	0.9846141
23	0.3446326	0.4925192	0.7948780	0.9678178
24	0.2836193	0.3888995	0.6270748	0.9112726
25	0.1255316	0.2336821	0.5659565	0.9057126
26	0.3194456	0.4384223	0.7349284	0.9562967
27	0.1619486	0.2316790	0.5043296	0.8842176
28	0.0454515	0.0671703	0.1817353	0.6220738
29	0.0707576	0.0894588	0.2229997	0.7032917

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12 0.9998232 0.9999467 1.0000002 1.0000000
13 0.9929863 0.9979154 0.9999822 1.0000000
14 0.9867029 0.9956160 0.9994421 1.0000000
15 0.9730106 0.9899829 0.9986633 0.9995319
16 0.9534453 0.9800016 0.9969724 0.9992313
17 0.9325560 0.9675105 0.9951763 0.9995215
18 0.9191875 0.9565970 0.9934598 0.9992332
19 0.8947805 0.9357861 0.9884437 0.9986417
20 0.8257973 0.8779652 0.9702530 0.9963423
21 0.7159785 0.8345258 0.9583384 0.9947432
22 0.8284063 0.8858284 0.9684628 0.9960505
23 0.7516755 0.8123697 0.9291257 0.9894163
24 0.6926874 0.7391886 0.8604153 0.9724589
25 0.4561008 0.5512760 0.7705901 0.9559797
26 0.9369271 0.9590048 0.9854876 0.9979031
27 0.8375972 0.8640408 0.9309466 0.9866180
28 0.7233153 0.7644902 0.8566202 0.9592480
29 0.9254403 0.9398230 0.9742375 0.9951715

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12 0.9991587 0.9997716 0.9999526 0.9999794
13 0.9686357 0.9908997 0.9979945 0.9990163
14 0.9469154 0.9839748 0.9973225 0.9995362
15 0.9080263 0.9677835 0.9945433 0.9983248
16 0.8385513 0.9362347 0.9907270 0.9985850
17 0.7654059 0.8952977 0.9845985 0.9977483
18 0.7010735 0.8513324 0.9775737 0.9977076
19 0.6114407 0.7802261 0.9623126 0.9956007
20 0.5042196 0.6814037 0.9317039 0.9916127
21 0.3199653 0.5675337 0.8925292 0.9860841
22 0.3271319 0.5778309 0.8942109 0.9871229
23 0.2514957 0.4698967 0.8241558 0.9752529
24 0.1782266 0.3279704 0.6786517 0.9394147
25 0.1260438 0.2622594 0.6274137 0.9299870
26 0.2175988 0.4300754 0.7975954 0.9710605
27 0.1447295 0.2696962 0.6245209 0.9279381
28 0.0655802 0.1212090 0.3478988 0.7794704
29 0.1315142 0.1831188 0.4248639 0.8297260

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12 0.9993849 0.9998407 0.9999801 1.0000000
13 0.9756160 0.9934611 0.9990649 0.9999844
14 0.9583364 0.9876474 0.9982128 0.9996610
15 0.9304619 0.9769028 0.9966459 0.9993678
16 0.8841143 0.9560008 0.9932181 0.9984165
17 0.9392892 0.9336476 0.9909130 0.9992461
18 0.7771371 0.8941364 0.9834737 0.9973751
19 0.7004296 0.8389016 0.9734232 0.9970182
20 0.6071070 0.7563303 0.9495235 0.9939580
21 0.4773484 0.7216459 0.9423940 0.9933401
22 0.5082797 0.7114187 0.9311245 0.9917875
23 0.4099379 0.6268937 0.8922460 0.9856854
24 0.3241130 0.4720875 0.7432757 0.9509617
25 0.2355933 0.4789025 0.8304743 0.9746722
26 0.2604444 0.4548163 0.8027778 0.9716999
27 0.2087221 0.3429592 0.6772486 0.9398842
28 0.0696485 0.1249755 0.3499751 0.7799608
29 0.1522037 0.2055245 0.4504889 0.8430598

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INELASTIC MATRIX DATA SET 6. MATERIAL 1104

0.5400E 00	0.6748E 00	0.8941E 00	0.1193E 01	0.1154E 01	0.9490E 00	0.8461E 00	0.6018E 00
0.4104E 00	0.3341E 00	0.2752E 00	0.1746E 00	0.3673E-01	0.	0.	0.
0.3457E-01	0.8074E-01	0.2561E 00	0.4457E 00	0.4929E 00	0.3731E 00	0.2365E 00	0.2481E 00
0.2073E 00	0.1390E 00	0.1538E 00	0.2002E 00	0.1041E 00	0.1301E-01	0.	0.
0.6560E-01	0.2269E 00	0.3238E 00	0.2757E 00	0.2691E 00	0.2129E 00	0.5845E-01	0.3196E-02
0.9317E-01	0.3848E-01	0.	0.	0.2462E-01	0.1579E-01	0.	0.
0.1743E 00	0.3778E 00	0.3677E 00	0.2200E 00	0.8839E-01	0.7750E-01	0.3520E-01	0.3063E-03
0.2974E-02	0.2066E-01	0.9684E-03	0.	0.	0.6122E-02	0.	0.
0.2227E 00	0.3571E 00	0.2717E 00	0.1303E 00	0.5236E-01	0.3301E-01	0.1780E-01	0.1041E-03
0.4173E-05	0.6581E-02	0.2143E-02	0.	0.	0.2892E-02	0.7507E-03	0.
0.1775E 00	0.2353E 00	0.1534E 00	0.6412E-01	0.2072E-01	0.1183E-01	0.8938E-02	0.2280E-04
0.5428E-05	0.5494E-03	0.1125E-02	0.	0.	0.4520E-03	0.5193E-03	0.
0.1051E 00	0.1237E 00	0.7330E-01	0.2817E-01	0.6740E-02	0.5127E-02	0.4309E-02	0.9963E-03
0.2898E-05	0.9218E-04	0.1735E-03	0.	0.	0.	0.1148E-04	0.
0.5173E-01	0.5662E-01	0.3163E-01	0.1154E-01	0.2583E-02	0.1207E-02	0.5262E-03	0.5892E-03
0.	0.5877E-04	0.9464E-04	0.	0.	0.	0.	0.
0.2273E-01	0.2379E-01	0.1282E-01	0.4534E-02	0.9610E-03	0.4484E-03	0.2935E-03	0.1922E-03
0.5258E-06	0.2857E-04	0.	0.	0.	0.	0.	0.
0.9314E-02	0.9489E-02	0.5002E-02	0.1736E-02	0.3491E-03	0.4635E-04	0.5310E-05	0.
0.	0.	0.1707E-04	0.	0.	0.	0.	0.
0.3659E-02	0.3667E-02	0.1907E-02	0.6541E-03	0.1370E-03	0.3539E-04	0.1072E-05	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.1461E-02	0.1390E-02	0.7170E-03	0.2442E-03	0.4846E-04	0.	0.	0.4397E-07
0.	0.	0.	0.	0.	0.	0.	0.
0.5279E-03	0.5206E-03	0.2673E-03	0.9063E-04	0.1793E-04	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.1971E-03	0.1936E-03	0.9911E-04	0.3352E-04	0.6621E-05	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.7315E-04	0.7170E-04	0.3664E-04	0.1237E-04	0.2441E-05	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.4237E-04	0.4195E-04	0.2140E-04	0.7220E-05	0.1424E-05	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.

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N2N MATRIX - DATA SET 7 MATERIAL 1104

0.4195E-04	0.2540E-05	0.
0.1698E-02	0.3044E-04	0.
0.1308E-01	0.1032E-03	0.
0.3376E-01	0.1534E-03	0.
0.4235E-01	0.1343E-03	0.
0.3338E-01	0.8424E-04	0.
0.1962E-01	0.4295E-04	0.
0.9619E-02	0.1928E-04	0.
0.4215E-02	0.8004E-05	0.
0.1725E-02	0.3169E-05	0.
0.6770E-03	0.1219E-05	0.
0.2590E-03	0.4608E-06	0.
0.9759E-04	0.1723E-06	0.
0.3642E-04	0.6403E-07	0.
0.1352E-04	0.2370E-07	0.
0.7922E-05	0.1386E-07	0.

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2. MUG FILE

The output MUG file contains a file directory, file specifications, and cross sections for each material. This file is described below.

A. MUG File Format and Contents

The MUG file is blocked at 128 words. The MUG file system allows for more than one file on a tape, however TDOWN generates only one file per tape. The first two blocks described below provide for multi-file tapes.

BLOCKS 1-2 Tape Dictionary

<u>Word(s)</u>	<u>Contents</u>
1	Tape ID name (6 characters)
2-61	Two words per file, the first a control word and the second contains the file name.

BLOCKS 3 Data for file

<u>Word(s)</u>	<u>Contents</u>
1	f, file name (5 characters)
2	I, number of lethargy groups
3	J, number of inelastic groups
4	N, number of materials in file
5	MDS, maximum number of groups any material can downscatter
6, N+5	The material numbers in order they appear on the file

BLOCK 4 Chi values for file

<u>Word(s)</u>	<u>Contents</u>
1,I	$(\chi_i \quad i = 1, I)$

BLOCK 5 Lethargy structure of file

<u>Word(s)</u>	<u>Contents</u>
1,I	$(\Delta u_i \quad i = 1, I)$

BLOCK 6+* Inelastic scattering matrix for material m

<u>Word(s)</u>	<u>Contents</u>
1+	$[(\sigma_{in})_{i \rightarrow j, m} \quad j = i+1, k], i=1, J-1]$ where $K = MDS+1$ when $1 \leq J-MDS$ $K = J$ when $i > j-MDS$

BLOCK 7+ Cross Sections for material m

<u>Word(s)</u>	<u>Contents</u>
1+	$[(\sigma_{tr})_{i, m}, (\sigma_f)_{i, m}, (\sigma_c)_{i, m}, (\sigma_{er})_{i, m},$ $(\sigma_{in})_{i, m} \text{ or } (\sigma_{sh})_{i, m}, v_{i, m}, i=1, I], m$

The format described in BLOCKS 6+ and 7+ are repeated for each material in the file.

LAST BLOCK

<u>Word(s)</u>	<u>Contents</u>
1	9999
2	0
3	0
4	0

*The "+" sign means the contents described may require more than one block.

The symbols used are defined as follows:

<u>SYMBOL</u>	<u>DEFINITION</u>
I	Number of lethargy groups
χ_i	The fraction of neutrons released by fission in Group i
Δu_i	Width of lethargy Group i
$(\sigma_{in})_{i \rightarrow j, m}$	Inelastic scattering from Group i to Group j for Material m (barns)
$(\sigma_{tr})_{i, m}$	Transport cross section for group i and Material m (barns)
$(\sigma_f)_{i, m}$	Fission cross section
$(\sigma_c)_{i, m}$	Capture cross section
$(\sigma_{er})_{i, m}$	Elastic removal cross section
$(\sigma_{in})_{i, m}$	Inelastic removal cross section
$(\sigma_{sh})_{i, m}$	Hydrogen scattering cross section from Group i ($990 \leq m \leq 999$)
$\nu_{i, m}$	Number of neutrons released per fission in Group i by Material m
m	Material number
N	Number of materials in file (maximum $N \leq 120$)
MDS	The maximum number of groups that down scattering is possible from any group

A sample listing of the contents of a MUG file is included in Section 7.2 of this report.

APPENDIX B

THE SELENGUT-GOERTZEL METHOD OF CALCULATING THE
ELASTIC SCATTERING MATRIX FOR HYDROGEN

When a neutron suffers an elastic collision with a hydrogen atom, its energy after collision can be anywhere between its initial energy and zero energy. If it is assumed that the scattering is isotropic in the center of mass system, the scattered neutron has equal probability of attaining any lower energy.

Assume that a neutron with energy E' is in energy Group i (with lower and upper energy limits E_i and E_{i-1} , respectively) and suffers a collision with a hydrogen atom. Also assume that the flux in Group i can be approximated by a $1/E$ variation. The probability that the scattered neutron attains an energy less than E_i is E_i/E' ; and the flux-averaged probability that a neutron is scattered out of group i is then:

$$(F_i)_{\text{avg}} = \frac{\int_{E_i}^{E_{i-1}} \frac{E_i}{E'} \frac{dE'}{E'}}{\int_{E_i}^{E_{i-1}} \frac{dE'}{E'}} = \frac{1 - e^{-\Delta u_i}}{\Delta u_i} \quad (1)$$

where Δu_i = lethargy width of Group i . The S-G removal cross section for Group i is then:

$$(\Sigma_{\text{SG}})_i = N_m (\sigma_{\text{sh}})_{m,i} \frac{1 - e^{-\Delta u_i}}{\Delta u_i} \quad (2)$$

where

$$\begin{aligned} N_m &= \text{Nuclear density of hydrogen} \\ (\sigma_{\text{sh}})_{m,i} &= \text{Scattering cross section for hydrogen in Group } i \end{aligned}$$

We can now compute the transfer cross section from Group i to Group j by calculating the probability that a neutron scattered out of Group i attains an energy greater than E_j , but less than E_{j-1} . (see Figure A).

The flux-averaged probability that a neutron scattered in Group i attains an energy less than E_{j-1} is:

$$(F_{j-1})_{\text{avg}} = \frac{\int_{E_i}^{E_{i-1}} \frac{E_{j-1}}{E'} \frac{dE'}{E'}}{\int_{E_i}^{E_{i-1}} \frac{dE'}{E'}} = \frac{e^{-\Delta u_l} (1 - e^{-\Delta u_i})}{\Delta u_i}, \quad (3)$$

and the averaged probability that the neutron is scattered past energy E_j is:

$$(F_j)_{\text{avg}} = \frac{\int_{E_i}^{E_{i-1}} \frac{E_j}{E'} \frac{dE'}{E'}}{\int_{E_i}^{E_{i-1}} \frac{dE'}{E'}} \left[\frac{e^{-\Delta u_j} (1 - e^{-\Delta u_i})}{\Delta u_i} \right] e^{-\Delta u_l} \quad (4)$$

Thus, the probability that a neutron scattered in Group i lands in energy Group j is:

$$F_j = (F_{j-1})_{\text{avg}} - (F_j)_{\text{avg}} = \frac{1 - e^{-\Delta u_i}}{\Delta u_i} (1 - e^{-\Delta u_j}) e^{-\Delta u_l}, \quad (5)$$

and the transfer cross section is:

$$(\Sigma_{SG})_{i \rightarrow j} = N_m (\sigma_{sh})_{m,i} \frac{1 - e^{-\Delta u_i}}{\Delta u_i} (1 - e^{-\Delta u_j}) e^{-\Delta u_l} \quad (6)$$

where

$$e^{-\Delta u_l} = e^{-\sum_{n=i+1}^{j-1} \Delta u_n}$$

FIGURE A

$$U_i = \ln \frac{E_o}{E_i}, \quad E_i = E_o e^{-U_i}$$

$$\Delta u_i = \ln \frac{E_{i-1}}{E_i}$$

APPENDIX C

PUNT - A CODE FOR CORRECTING, MERGING,
AND LISTING GMUG FILES

The computer code PUNT allows the user to:

- a. Combine two or more (<9) GMUG files,
- b. Delete class data sets from a GMUG file,
- c. Overlay any word(s) in a class data set,
- d. List any class data set.

All of the above capabilities of the code can be combined in a single case.

INPUT DESCRIPTION

A. Control cards

The following control cards are necessary for running PUNT on the GE635 computer:

<u>Card Purpose</u>	<u>Contents</u>		
	Column:	1	8 16
Job Identification	\$	IDENT	cccc,III-locat,PUNT
Sets FORTRAN Options in the loader	\$	OPTION	FORTRAN
Program Execute Command	\$	EXECUTE	
Program Limits	\$	LIMITS	tt,29K,9K,10000

<u>Card Purpose</u>	<u>Contents</u>		
	Column:	1	8 16
The FFILE cards define files where block data is transferred without using buffers. A FFILE card is input for every tape. The file code* number (Columns 16, 17) establish the correspondence between the TAPE and FFILE cards	\$	FFILE	01,NBUFFS/0
Output Tape	\$	TAPE	01,G1DR,,,NEW GMUG
The input tapes are on file codes starting with 11 through a maximum of 19	\$	TAPE	11,G11DD,,MMMM,,GMUG
File for printed output	\$	SYSOUT	06
Transliteration Card	\$	INCODE	IBMF
Job Conclusion Card	\$	ENDJOB	

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

The FORTRAN source deck or binary deck is inserted between the OPTION and EXECUTE cards. The Data cards are inserted between the INCODE and ENDJOB cards.

*File code numbers are used on all FFILE, TAPE, FILE and SYSOUT cards. These are the numbers used by the program to reference a particular peripheral file.

B. Data Cards

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

	Columns:	1	28
CASE card		)PUNTHH*cccc	DDDDDD
LAST card		)LAST	

HHH = user's initials	} optional
cccc = case identification	
DDDDDD = date	

Each input data card is identified by a card type which may be either an instruction or a location card. A location card, which will later be called card type "DATACL", identifies the data class set for the executing preceding instruction. All instruction cards are optional except the TAPES and LAST cards.

The card type name is input in columns 1-6 (left justified).
Data on the cards is input in free format* in columns 21-80.

CARD TYPES USED BY PUNT

TAPES - The number of input tapes are specified on this card (<9)

<u>Columns</u>	<u>Content</u>
1-6	TAPES
21-80	DATA - number of input tapes (integer)

DELETE - An entire data class set on a particular input tape is deleted by the use of this card (optional). This instruction will be executed before input files are merged.

* See rules 2a, b, c, d, of NIPS format, Section 5.

<u>Columns</u>	<u>Content</u>
1-6	DELETE
21-80	Data - IF,6HDATACL where IF = The input tape file code number minus 10 (integer) DATACL = The data class set to be deleted (Hollerith)

MODIFY - Any data on the GMUG file may be altered by a MODIFY card with location cards following it. Modification is done on the merged GMUG file.

<u>Columns</u>	<u>Content</u>
1-6	MODIFY
21-80	Data - 6HDATACL, identifies the data class set to be modified. (Hollerith)

DATACL - This card follows the MODIFY card and contains the data modifications.

<u>Columns</u>	<u>Content</u>
1-6	Data Class set indicated on MODIFY card (integer)
21-80	Data - $I, D_I, D_{I+1} \dots$ I is the location in the data set array to start modifying data. (integer) In determining I, multi-dimensioned arrays must be considered as a one- dimensional array. $D_I, D_{I+1} \dots$ are the new data for the array. (Integer, floating point or Hollerith depending on data) A maximum of 15 values per card is allowed.

LIST - This card selects the list option in the program. The data class(es) listed are those on the merged GMUG file.

<u>Columns</u>	<u>Content</u>
1-6	LIST

DATACL - Following the LIST card, this card specifies the data set to be listed

<u>Columns</u>	<u>Content</u>
1-6	Data class set to be listed

LAST - This card indicates no more instructions follow.

<u>Columns</u>	<u>Content</u>
1-6	LAST

CODE PROCEDURE

The first step in PUNT is to delete all unwanted data sets on the input files. The files are then merged to generate the output GMUG file. The file data containing the group structure is obtained from the first input tape. The file directory containing the number and identification of the data class sets is generated by the code. Data classes are obtained from all the input files and duplicate data classes, if any, are overlaid by the last input tape (tape with largest file code number) containing the data class.

APPENDIX D

HETEROGENEITY CORRECTION TO THE SELF-SHIELDING
CROSS SECTION PARAMETER, σ_o

The heterogeneity correction to the self-shielding parameter, σ_o , is based upon the rational approximation which was formulated by Bell.⁽³⁾ This approximation introduces a term to account for the mean free path in a simple, two region cell model such as shown in Figure 2. The Bell approximation is expressed as

$$\begin{aligned}
 (\sigma_o)_{i,m}^{\text{eff}} &= (\sigma_o)_{i,m} + \tau_m / N_{m,1} \\
 &= \frac{\Sigma'_{i,1} - N_{m,1} (\sigma_T)_{i,m}}{N_{m,1}} + \frac{S/4V_1}{N_{m,1} (1 + S/4V_2 \Sigma'_{i,2})}
 \end{aligned}
 \tag{D.1}$$

where $\Sigma'_{i,1}$ and $\Sigma'_{i,2}$ = the total macroscopic cross sections in regions 1 and 2 respectively.

$$\Sigma'_{i,1} = \sum_n N_{n,1} (\sigma_t)_{i,n}$$

$$\Sigma'_{i,2} = \sum_n N_{n,2} (\sigma_t)_{i,n}$$

V_1 and V_2 = the volumes of regions 1 and 2 respectively.

$N_{n,1}$ and $N_{n,2}$ = the atom concentrations of the n-th material in regions 1 and 2 respectively.

- S = the surface area of region 1
 $(\sigma_t)_{i,n}$ = the total microscopic cross section for the i -th group and n -th material, and
 $\sum_n$ = summation over all materials in a given composition

Equation D.1 can be reduced to a particular geometry and smeared atom concentrations by making the following substitutions.

Cylindrical Cell

$$N_{n,1} = N_n \frac{D_2^2}{D_1^2}$$

$$\Sigma'_{i,1} = \left[\sum_n f_n N_n (\sigma_t)_{i,n} \right] \frac{D_2^2}{D_2^2 - D_1^2} = (\Sigma_{i,1}) \frac{D_2^2}{D_1^2}$$

$$\Sigma'_{i,2} = \left[\sum_n (1 - f_n) N_n (\sigma_t)_{i,n} \right] \frac{D_2^2}{D_2^2 - D_1^2} = (\Sigma_{i,2}) \frac{D_2^2}{D_2^2 - D_1^2}$$

$$S/4V_1 = 1/D_1$$

$$S/4V_2 = D_1 / (D_2^2 - D_1^2)$$

Plate Cell

$$N_{n,1} = N_n \frac{D_2}{D_1}$$

$$\Sigma'_{i,1} = \left[\sum_n n N_n (\sigma_t)_{i,n} \right] \frac{D_2}{D_1} = \Sigma_{i,1} \frac{D_2}{D_1}$$

$$\epsilon'_{i,2} = \left[\sum_n (1-n_n) N_n (\sigma_t)_{i,n} \right] \frac{D_2}{D_2 - D_1} = \epsilon_{i,1} \left(\frac{D_2}{D_2 - D_1} \right)$$

$$S/4V_1 = 1/2 D_1$$

$$S/4V_2 = 1/2(D_2 - D_1)$$

where N_m is the smeared atom concentration in the cell.

D and D_2 are the dimension from Figure 2, and f_n is the fraction of the n -th material in region 1.

Carrying out the indicated substitutions and rearranging we get

Cylindrical Cell

$$(\sigma_o)_{i,m}^{\text{eff}} = \frac{\epsilon_{i,1}}{N_m} - (\sigma_T)_{i,m} + \frac{1}{N_m \left(\frac{D_2^2}{D_1} + \frac{1}{\epsilon_{i,2}} \right)} \quad \text{D.2}$$

and,

Plate Cell

$$(\sigma_o)_{i,m}^{\text{eff}} = \frac{\epsilon_{i,1}}{N_m} - (\sigma_T)_{i,m} + \frac{1}{N_m \left(2D_2 + \frac{1}{\epsilon_{i,2}} \right)} \quad \text{D.3}$$

APPENDIX E

TAYLOR SERIES EXPANSION AND INTERPOLATION OF
SELF-SHIELDING f-FACTORS

The Taylor series expansion and the interpolation of the self-shielding f-factors are based upon the simple schematic diagram given below.

Here f_k is a function of X_k and Δ is the distance (a constant) between successive values of X_k . We wish to determine the value of f at X .

The self-shielding coefficient, f , is first expanded about the two neighboring points, f_k and f_{k+1} , by carrying along the first three terms of the Taylor series. Thus

$$f @ f_k = f_k + f'_k \left(\frac{\delta_1}{\Delta} \right) + \frac{f''_k}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \quad \text{E.1}$$

$$f @ f_{k+1} = f_{k+1} + f'_{k+1} \left(\frac{\delta_2}{\Delta} \right) + \frac{f''_{k+1}}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \quad \text{E.2}$$

where f'_k and f''_k = the first and second derivatives respectively
of f_k

f'_{k+1} and f''_{k+1} = the first and second derivatives respectively
of f_{k+1}

$$\delta_1 = X - X_k$$

$$\delta_2 = X - X_{k+1}$$

The derivatives of f_k are defined as follows:

$$f'_k = \frac{f_{k+1} - f_{k-1}}{2} \quad \text{E.3}$$

$$f''_k = f_{k+1} - 2f_k + f_{k-1} \quad \text{E.4}$$

Similar expressions are used for f_{k+1} with the values of k increased by 1.

A simple weighting of the two expansion series is used to determine f . That is

$$f = \frac{\delta_1}{\Delta} \left[f @ f_{k+1} \right] - \frac{\delta_2}{\Delta} \left[f @ f_k \right] \quad \text{E.5}$$

Substituting Equations E.1, E.2, E.3 and E.4 into Equation E.5 and rearranging gives the following

$$f = \frac{\delta_1}{\Delta} \left[f_{k+1} \left(1 - \left(\frac{\delta_2}{\Delta} \right)^2 \right) + f_k \left(-\frac{\delta_2}{2\Delta} + \frac{1}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \right) + f_{k+2} \left(\frac{\delta_2}{2\Delta} + \frac{1}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \right) \right] \\ - \frac{\delta_2}{\Delta} \left[f_k \left(1 - \left(\frac{\delta_1}{\Delta} \right)^2 \right) + f_{k-1} \left(-\frac{\delta_1}{2\Delta} + \frac{1}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \right) + f_{k+1} \left(\frac{\delta_1}{2\Delta} + \frac{1}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \right) \right] \quad \text{E.6}$$

Two special cases must be considered. First, for $X_{k_{\min}} < X \leq X_{k_{\min}+1}$, where $k_{\min}$ is the indicator of the lowest value of the X_k 's, only the Taylor expansion around $X_{k_{\min}+1}$ is used. Therefore, substituting Equations E.3 and E.4 into Equation E.2 and rearranging gives,

$$f = f_{k_{\min}+1} \left[1 - \left(\frac{\delta_2}{\Delta} \right)^2 \right] + f_{k_{\min}} \left[-\frac{\delta_2}{2\Delta} + \frac{1}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \right] + f_{k_{\min}+2} \left[\frac{\delta_2}{2\Delta} + \frac{1}{2} \left(\frac{\delta_2}{\Delta} \right)^2 \right] \quad E.7$$

The second special case occurs when X falls between $X_{k_{\max}}$ and $X_{k_{\max}} + \Delta$, where $k_{\max}$ is the indicator for the largest value of the X_k 's. For this case, only the Taylor expansion $f_{k_{\max}}$ is used and $f_{k_{\max}+1}$ is set equal to 1. Substituting Equations E.3 and E.4 into Equation E.1 gives

$$f = f_{k_{\max}} \left[1 - \left(\frac{\delta_1}{\Delta} \right)^2 \right] + f_{k_{\max}-1} \left[-\frac{\delta_1}{2\Delta} + \frac{1}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \right] + \left[\frac{\delta_1}{2\Delta} + \frac{1}{2} \left(\frac{\delta_1}{\Delta} \right)^2 \right] \quad E.8$$

APPENDIX F

USER ERROR INDEX

<u>Error No.</u>	<u>Meaning</u>
103	A GMUG material was not found on the GMUG file.
104	A required input class is missing.
105	The number of groups found on the GMUG file do not agree with the users input. (CLASS 2 WORD 1)
113	The referenced composition in CLASS 32 does not contain the material.
114	A material in CLASS 5 was not found in CLASS 32.
121	MUG file downscatter is greater than the last group allowed a source term. (CLASS 2 WORDS 14 and 15).
122	Last group on MUG file to have a source term is greater than the number of groups. (CLASS 2 WORD 14)
120	Geometry in the x and y direction cannot both be cylindrical (CLASS 2 WORDS 4 and 6).
111	Too many output (MUG) materials. (Limit is 120) (Check CLASS 32).
112	No materials found in CLASS 32. Search ends at the first zero material found. (Error Nos. 131-160 occur in specifying the flux solutions)
131	Number of iterations is ≤ 0 .
132	Delta-K convergence is ≤ 0.0
133	Estimate of leakage is ≤ 0.0 .
134	Second leakage value is ≤ 0.0
135	A boundary condition set number is ≤ 0 .
136	Negative total removal option is not 0.1 or 2.
137	Negative flux option is not 0.1 or 2.
138	Buckling set number is not defined.

<u>Error No.</u>	<u>Meaning</u>
139	Region numbers for flux solutions are incorrect. (CLASS 7 WORDS 1 and 2).
141	Number of intervals is ≥ 1000 or ≤ 1 . (CLASS 3)
142	Radius of a region $\leq$ to the previous region. (CLASS 3).

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