# TRANSX 2: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes

R. E. MacFarlane

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# TRANSX 2: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes

by

#### R. E. MacFarlane

#### ABSTRACT

TRANSX 2.0 is a computer code that reads nuclear data from a library in MATXS format and produces transport tables compatible with many discrete-ordinates  $(S_N)$  and diffusion codes. Tables can be produced for neutron, photon, charged-particle, or coupled transport. Options include adjoint tables, mixtures, homogeneous or heterogeneous self-shielding, group collapse, homogenization, thermal upscatter, prompt or steady-state fission, transport corrections, elastic removal corrections, and flexible response function edits. This report describes version 2.0 of TRANSX, which was prepared in January of 1992.

#### I. INTRODUCTION

Discrete-ordinates  $(S_N)$  transport codes, which solve the Boltzmann equation for the distribution of neutrons and photons in nuclear systems, have reached a high level of development. The early one-dimensional codes DTF-IV<sup>1</sup> and ANISN<sup>2</sup> are very widely used. The development of diffusion acceleration<sup>3</sup> as well as increasing computer speed and capacity has made detailed transport calculations more economical; as a result, codes such a ONEDANT<sup>4</sup> and TWODANT<sup>5</sup> are seeing increasing use. The toroidal geometry capability of TRIDENT-CTR<sup>6</sup> and its successor TRISM<sup>7</sup> are very useful for fusion reactor analysis. The DIF-3D<sup>8</sup> diffusion code and Monte-Carlo codes with multigroup capability like MCNP<sup>9</sup> are also used frequently.

However, many of the users of transport codes have the same complaint: it is hard to get good, up-to-date, documented cross-section data and prepare them for input into these codes. The difficulties are multiplied if there is anything unusual

about the problem, such as fine groups, self-shielding, transport cross sections, or sophisticated response edits (e.g., heating, damage, or gas production). This report describes a utility code called TRANSX (for transport cross-section code) that works together with a generalized cross-section library called MATXS (for material cross-section library) to give the transport code user easier access to appropriate nuclear data and some capabilities difficult or impossible to get with any other system.

The version of TRANSX described in this report can be used to construct data for fusion reactors, fast fission reactors, thermal fission reactors, and shielding problems. Its main weakness is in computing resonance effects in thermal reactors.

TRANSX was originally developed in the late seventies to handle cross sections for fission, fusion, and shielding applications at Los Alamos. In the early eighties, extensions to handle heterogeneous self-shielding problems for fast reactors were added. In 1984, a version without the fast reactor features was released as TRANSX-CTR. 10 It was especially well-suited for problems in controlled thermonuclear research (CTR) because of its ability to prepare coupled tables and response edits for heating, damage, gas production, and delayed activity. Various later versions have been made available without formal release or complete documentation; for example, Version 1.11 has been available as S11 at Los Alamos, on the Magnetic Fusion Energy (MFE) computer system at Livermore, and on the San Diego Super Computer Center system since late 1987. Version 1.13, which includes charged-particle capabilities, has been used extensively at Los Alamos. This gradual accumulation of changes and new capabilities, plus the need to react to a new version of the MATXS format developed for NJOY 91, plus the need for a fully documented code more consistent with modern Quality Assurance (QA) requirements, has led to the creation of this new version.

Section II of this report discusses the data needs of the typical  $S_N$  codes and describes the theoretical background; Section III gives detailed examples of a wide variety of problems that can be solved using TRANSX; Section IV contains descriptions of the input and output files used by TRANSX, including the MATXS cross-section library; Section V summarizes several available MATXS libraries; and Section VI gives a detailed discussion of the code aimed at programmers who have to convert, modify, or maintain the code. Several appendices are attached that give the format specifications for the input and output interface files and partial listings of the outputs from the sample problems.

#### II. DATA NEEDS OF TRANSPORT CODES

The  $S_N$  transport codes solve the equation  $^{11}$ 

$$\mu \frac{\partial}{\partial x} \phi_g(\mu, x) + \sigma_g^{SN}(x) \phi_g(\mu, x) = \sum_{\ell=0}^N P_{\ell}(\mu) \sum_{g'} \sigma_{\ell g \leftarrow g'}^{SN}(x) \phi_{\ell g'} + S_g(\mu, x) , \quad (1)$$

where one-dimensional plane geometry has been used for simplicity,  $\mu$  is the scattering cosine, x is position,  $\phi(\mu, x)$  is the angular flux for group g,  $\phi_{lg}$  is the Legendre flux for group g,  $P_{\ell}(\mu)$  is a Legendre polynomial, and  $S_g(\mu, x)$  is the external and fission source into group g. The cross sections in Eq. (1) must be defined to make  $\phi_g$  as close as possible to the solution of the Boltzmann equation. As shown in the reference, <sup>11</sup> the multigroup Boltzmann equation can be written in the  $P_N$  form:

$$\mu \frac{\partial}{\partial x} \psi(\mu, x) + \sum_{\ell=0}^{N} P_{\ell}(\mu) \, \sigma_{\ell t g}^{PN}(x) \, \psi_{\ell g} = \sum_{\ell=0}^{N} P_{\ell}(\mu) \sum_{g'} \sigma_{\ell g \leftarrow g'}^{PN}(x) \, \psi_{\ell g'} + S_g(\mu, x) , \quad (2)$$

where the P<sub>N</sub> cross sections are given by the following group averages:

$$\sigma_{\ell tg}^{PN} = \frac{\int_g \sigma_t(E) W_{\ell}(E) dE}{\int_g W_{\ell}(E) dE} \quad , \tag{3}$$

and

$$\sigma_{\ell g \leftarrow g'}^{PN} = \frac{\int_{g'} dE' \int_g dE \, \sigma_\ell(E' \rightarrow E) W_\ell(E')}{\int_{g'} dE' W_\ell(E')} \quad . \tag{4}$$

In these formulas,  $\sigma_{\ell}(E)$  and  $\sigma_{\ell}(E' \to E)$  are the basic energy-dependent total and scattering cross sections, and  $W_{\ell}(E)$  is a weighting flux that should be chosen to be as similar to  $\psi$  as possible. As will be seen later, these  $P_N$  cross sections are available on the MATXS libraries produced by NJOY. 12, 13, 14, 15 When Eq. (2) is compared with Eq. (1), it is evident that the  $S_N$  equations require

$$\sigma_{\ell q \leftarrow q'}^{SN} = \sigma_{\ell q \leftarrow q'}^{PN} \quad \text{for } g' \neq g \quad , \tag{5}$$

and

$$\sigma_{\ell a \leftarrow a}^{SN} = \sigma_{\ell a \leftarrow a}^{PN} - \sigma_{\ell t a}^{PN} + \sigma_{a}^{SN} \quad , \tag{6}$$

where  $\sigma_g^{SN}$  is not determined. The choice of  $\sigma_g^{SN}$  gives rise to a "transport approximation" and various recipes are in use.

## A. Transport Approximations

It is convenient to write

$$\sigma_{\ell g \leftarrow g}^{SN} = \sigma_{\ell g \leftarrow g}^{PN} - (\sigma_{\ell tg}^{PN} - \sigma_{otg}^{PN}) - \Delta_g^N \quad , \tag{7}$$

and

$$\sigma_q^{SN} = \sigma_{otg}^{PN} - \Delta_q^N \quad . \tag{8}$$

The term in parentheses corrects for the anisotropy in the total reaction rate term of the Boltzmann equation, and  $\Delta_g^N$  can be chosen to minimize the effects of truncating the Legendre expansion at  $\ell=N$ . The recipes available in TRANSX are as follows:

## Consistent-P approximation:

$$\Delta_q^N = 0 \quad , \tag{9}$$

## Inconsistent-P approximation:

$$\Delta_g^N = \sigma_{otg}^{PN} - \sigma_{N+1,tg}^{PN} \quad , \tag{10}$$

Diagonal transport approximation:

$$\Delta_a^N = \sigma_{ota}^{PN} - \sigma_{N+1,ta}^{PN} + \sigma_{N+1,a\leftarrow a}^{PN} \quad , \tag{11}$$

Bell-Hansen-Sandmeier or extended transport approximation:

$$\Delta_g^N = \sigma_{otg}^{PN} - \sigma_{N+1,tg}^{PN} + \sum_{g'} \sigma_{N+1,g' \leftarrow g}^{PN} , \qquad (12)$$

and

Inflow transport approximation:

$$\Delta_g^N = \sigma_{otg}^{PN} - \sigma_{N+1,tg}^{PN} + \frac{\sum_{g'} \sigma_{N+1,g \leftarrow g'}^{PN} \phi_{N+1,g'}}{\phi_{N+1,g}} . \tag{13}$$

The first two approximations are most appropriate when the scattering orders above N are small. The inconsistent option removes most of the delta-function

of forward scattering introduced by the correction for the anisotropy in the total scattering rate and should normally be more convergent than the consistent option. For libraries produced with an  $\ell$ -independent flux guess and in the absence of self-shielding, the difference between "consistent" and "inconsistent" vanishes.

The diagonal and Bell-Hansen-Sandmeier (BHS) recipes make an attempt to correct for anisotropy in the scattering matrix and are especially effective for forward-peaked scattering. The BHS form is most often used, but the diagonal option can be substituted when BHS produces negative values.

The inflow recipe makes the N+1 term of the  $P_N$  expansion vanish, but it requires a good knowledge of the N+1 flux moment from some previous calculation. Inflow reduces to BHS for systems in equilibrium by detail balance (*i.e.*, the thermal region). The diffusion approximation obtained using the inflow formula is equivalent to a  $P_1$  transport solution.

These corrections require data from the (N+1)-th Legendre moments of the cross sections to prepare a corrected N-table set. The user of the TRANSX program should be certain that, in fact, (N+1) tables are available on the MATXS file when producing an N-table transport-corrected set. Absence of the (N+1) tables is not fatal, but obviously the cross sections will not contain the desired corrections.

#### B. Fission Source

The source of fission neutrons into a group is given by

$$S_g = \sum_{g'} \sigma_{fg \leftarrow g'} \,\phi_{0g'} \quad , \tag{14}$$

where  $\sigma_{fg \leftarrow g'}$  is the fission matrix that is available on the MATXS file. However, most existing transport codes do not use this matrix form because the upscatter is expensive to handle and a reasonably accurate alternative exists. Except for relatively high neutron energies, the spectrum of fission neutrons is only weakly dependent on initial energy. Therefore, the fission source can be written as

$$S_g = \chi_g \sum_{g'} \bar{\nu}_{g'} \, \sigma_{fg'} \, \phi_{0g'} \quad , \tag{15}$$

where  $\bar{\nu}_g$  is the fission neutron yield,  $\sigma_{fg}$  is the fission cross sections, and  $\chi_g$  is the average fission spectrum, which can be defined by

$$\chi_g = \frac{\sum_{g'} \sigma_{fg \leftarrow g'} \phi_{0g'}}{\sum_{g'} \bar{\nu}_{g'} \sigma_{fg'} \phi_{0g'}} , \qquad (16)$$

where the fission neutron production rate can also be written as

$$\sum_{g'} \bar{\nu}_{g'} \, \sigma_{fg'} \, \phi_{0g'} = \sum_{g} \sum_{g'} \sigma_{fg \leftarrow g'} \, \phi_{0g'} \quad . \tag{17}$$

Clearly,  $\chi_g$  as given by Eq. (16) depends on the flux in the system of interest. The dependence is weak except for high incident energies, and a rough guess for  $\phi_{0g}$  usually gives an accurate spectrum. When this is not the case, a sequence of calculations can be made, using the flux from each step to improve the  $\chi_g$  for the next step.

The matrix in a MATXS file represents the prompt part of fission only. Steady-state (SS) fission is obtained using two auxiliary pieces of data: delayed  $\bar{\nu}$  and delayed  $\chi$ . Therefore,

$$\bar{\nu}_{g'}^{SS}\sigma_{fg'} = \sum_{g} \sigma_{fg\leftarrow g'} + \bar{\nu}_{g'}^{D}\sigma_{fg'} \quad , \tag{18}$$

and

$$\chi_g^{SS} = \frac{\sum_{g'} \sigma_{fg \leftarrow g'} \phi_{0g'} + \chi_g^D \sum_{g'} \bar{\nu}_{g'}^D \sigma_{fg'} \phi_{0g'}}{\sum_{g} \sum_{g'} \sigma_{fg \leftarrow g'} \phi_{o0'} + \sum_{g'} \bar{\nu}_{g'}^D \sigma_{fg'} \phi'_{0g}} .$$
 (19)

For large group structures, the square fission matrices can consume a large part of the library. As already noted, the shape of the fission spectrum is not strongly dependent on initial energy. In fact, the shape is independent of energy at low energies. Therefore, the fission matrix can be split into slow and fast parts,

$$\sigma_{fg \leftarrow g'} = \chi_g^S (\bar{\nu}\sigma_f)_{g'}^S + \sigma_{fg \leftarrow g'}^F . \tag{20}$$

Starting with NJOY 91.0, the GROUPR module automatically determines the energy range over which the fission spectrum is constant, and it generates a production cross section and normalized spectrum for this range. At higher energies, it produces a rectangular fission matrix. The new version of the MATXS format

established for NJOY 91 uses a generalized format for transfer matrices that allows for this decomposition of a matrix into two vectors and a smaller matrix. TRANSX 2.0 can then reconstruct the full representation of fission using Eq. (20).

The fission representation for some materials may be divided into the separate reactions (n, f), (n, n'f), (n, 2nf), and (n, 3nf). Because the second-, third-, and fourth-chance fission channels are only open at high energies (for example, above 6 MeV for  $^{235}$ U), their corresponding fission matrices are always rectangular on the MATXS library and do not cause a space problem. In any case, the prompt fission source produced by TRANSX includes all of these partial matrices. This full matrix treatment is important for 14-MeV source problems (for example, fusion-fission hybrid design).

This approach gives TRANSX a very general and efficient fission source capability. The same library can be used to compute  $\chi$  for a fast or thermal system; in fact, if region fluxes are available,  $\chi$  for a given material can be different in each region of a problem.

## C. Transport Tables

The data required for an  $S_N$  flux solution using Eq. (1) have been shown to be

$$\sigma_g$$
,  $\sigma_{\ell g \leftarrow g'}$ ,  $\bar{\nu}_g \sigma_{fg}$ , and  $\chi_g$ ,

where the superscript SN has been omitted for simplicity. The  $S_N$  codes also traditionally use a particle-balance cross section (often loosely called "absorption") defined by

$$\sigma_{ag} = \sigma_g - \sum_{g'} \sigma_{0g' \leftarrow g} \quad . \tag{21}$$

This quantity is also computed by TRANSX by adding all the absorption reactions  $[(n, \gamma), \text{fission}, (n, p), (n, \alpha), \text{etc.}]$  and subtracting (n, 2n), twice (n, 3n), and so on. The two methods are formally equivalent, except that small numerical differences due to cross-section processing lead to unreasonable values for  $\sigma_{ag}$ , as computed from Eq. (21), when  $\sigma_{ag}$  is small with respect to  $\sigma_g$ . In such cases,  $\sigma_{ag}$  is replaced by the value from the direct calculation, and the  $\sigma_g$  position of the transport table is adjusted accordingly. Note that  $\sigma_{ag}$  can be negative if more particles are produced by (n, xn) reactions than are absorbed. Negative values occur in coupled sets as well, as will be seen below.

When the flux calculation is complete, it is often necessary to compute some response such as heating, radiation damage, gas production, photon production,

or dose to tissue. Therefore,  $S_N$  codes allow for reading several response-function edit cross sections,  $\sigma_{Eq}$ .

The original  $S_N$  codes read  $\chi$  as a special array, and the cross sections were arranged into "transport tables" by "position" as shown in Table 1. Note that the positions containing scattering data give all the source groups that scatter into the same final or "sink" group. Even the newer codes retain many features of this structure, and TRANSX input uses terminology based on the table.

A transport table like this is required for each group, Legendre order, and material. The tables may be "material ordered" or "group ordered".

Material ordering is the natural result of preparing a library from evaluated nuclear data. The MATXS files are material ordered. The tables are written onto a library with the outermost loop being material, then Legendre order, then group as the inner loop.

However, group ordering is the way the cross sections are needed in the codes. The  $S_N$  equations are solved by sweeping down from group 1 to the lower energy groups, so cross sections for all materials and orders are needed for each group in sequence. The library is ordered with group as the outermost loop, then Legendre order, then material. Of course, the  $S_N$  codes contain the logic to change the input library from material to group ordering if the entire cross-section set will fit into the available memory. If the group structure is too large for the internal logic, the group-ordered TRANSX output can be requested, thereby allowing very large group structures to be used for transport calculations. It may be noted that fusion-related transport calculations (other than hybrid studies) do not require iteration to converge a fission source, so they characteristically employ larger group structures than are practical with multiplying systems. Thus, this group-ordered option, as well as the adjoint option discussed below, may be of particular value in fusion.

#### D. Neutron-Photon Coupled Sets

The discrete-ordinates equation can be applied equally well to neutron and photon transport; it is only necessary to provide the appropriate neutron or photon cross sections for the transport tables. In both cases, downscatter predominates (excluding fission), and the equations can be solved by sweeping through the groups from high energy to low energy.

Since photon production from neutron reactions is usually stronger than photoneutron production, the same downscatter structure can be obtained by defining a

Position		Contents for Group $g$		
1 : NED	}	$\sigma_{Eg}$	Response edits	
NED+1 NED+2 NED+3		$\sigma_{ag}$ $ar{ u}_g\sigma_{fg}$ $\sigma_g$	Standard edits	
NED+4  : NED+NUP+3	}	$\sigma_{g \leftarrow g'}$	Upscatter $(g' > g)$	
NED+NUP+4		$\sigma_{g \leftarrow g'}$	In-group $(g' = g)$	
NED+NUP+5  : NTABL	}	$\sigma_{g \leftarrow g'}$	Downscatter $(g' < g)$	

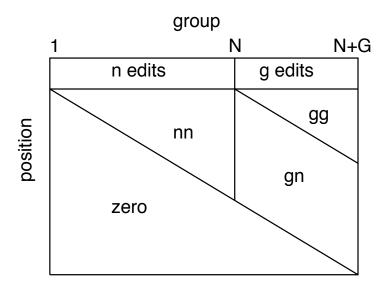
 $\mathbf{NED} \hspace{1cm} = \text{number of extra response edits (NED} \geq \hspace{-0.5cm} \geq \hspace{-0.5cm} 0)$ 

 $\begin{array}{ll} \mathbf{UP} & = \text{maximum number of upscatter groups } (0 \leq \text{NUP} \leq \text{NGROUP}) \\ \mathbf{NTABL} & = \text{table length } (\text{NED} + 4 + \text{NUP} \leq \text{NTABL} \leq \text{NED} + 4 + \text{NUP} + \text{NGROUP}) \\ \end{array}$ 

NGROUP = number of energy groups

**IPTOT** = NED+3 = position of total cross section

 Table 1: Transport Table Terminology



**Figure 1:** Arrangement of neutron (n) and photon (g) cross sections in a coupled transport table with no upscatter.

composite group structure with N neutron groups arranged as groups 1 through N, and G photon groups attached as groups N+1 through N+G. The arrangement is shown schematically in Fig. 1. Photoneutron production could be included with fission.

A coupled set provides the convenience of solving both the neutron and photon problems simultaneously with a single transport code run. Because more than one photon is normally produced by a neutron reaction (i.e., cascades), the particle-balance absorption edit  $\sigma_{ag}$  will usually be large and negative for a coupled set. Special features are available in some transport codes to allow the photon part of a response to be computed separately from the neutron part. As will be seen later, the GOXS interface format includes a parameter LNG to define the break point between the neutron and photon parts of the group structure.

## E. Charged-Particle Coupled Sets

This version of TRANSX is capable of producing transport tables for chargedparticle transport and coupled sets for more than two particles. The main difference between charged-particle cross sections and neutral-particle cross sections occurs for elastic scattering, because the Rutherford cross section becomes singular as the scattering angle goes to zero. In practice, this singularity is screened out by the electronic structure of the material. This is no longer a strictly nuclear problem, and the forward transport of charged particles is normally handled as a continuous slowing-down calculation using stopping powers. NJOY constructs charged-particle elastic matrices that include scattering to cosines less than 0.96 only (approximately  $20^{\circ}$ ).

Coupled transport is natural for charged-particle problems. High-energy neutrons normally produce secondary protons, and these protons can produce additional secondary neutrons. The structure of a coupled set for neutron-proton-photon transport is shown in Fig. 2. Note that a (p,n) reaction looks like an upscatter event in this type of table. The user must be careful to use NUP>0, and the transport calculation may run more slowly because it will have to use outer iterations.

## F. The Adjoint Problem

Solutions to the adjoint transport equation are useful for calculating the change in the response of a system to a small perturbation and for calculating the source that will give a desired response. Adjoint fluxes are being used more and more frequently to compute the sensitivity of a response to changes in the basic cross sections.

The adjoint transport equation can be obtained from the direct or forward equation discussed above by transposing the scattering and fission matrices. However, this converts the downscatter calculation into an upscatter calculation. If the order of the groups is then reversed, the cross sections can be used with the regular transport equation; the solution for the direction  $\vec{\Omega}$  is just the adjoint flux for direction  $-\vec{\Omega}$  numbered backwards.

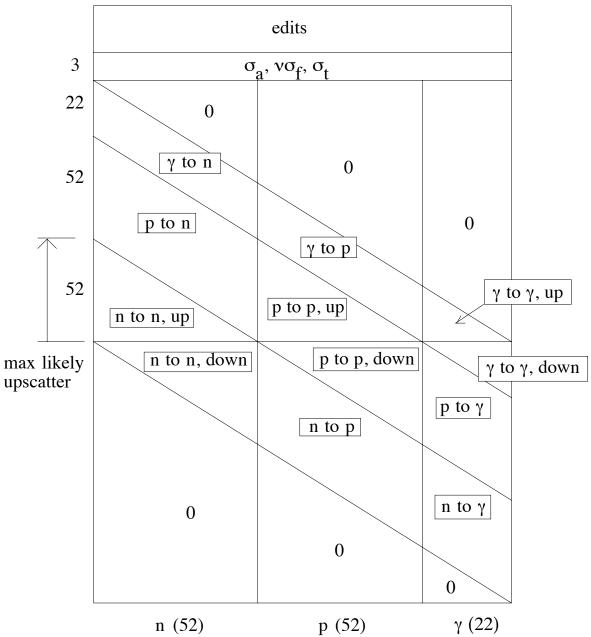
The existing  $S_N$  codes perform this operation of transposition and reordering of the groups, but only if the entire cross-section table fits into core storage at once. TRANSX can produce an adjoint set in group ordering, thereby allowing fine-group adjoint solutions to be obtained. When TRANSX adjoint tables are used, the  $S_N$  code must be run in forward mode, and the adjoint flux is obtained from the  $S_N$  flux solution  $\sigma(g, \vec{\Omega})$  using

$$\phi^{+}(g,\vec{\Omega}) = \phi(N-g+1,-\vec{\Omega})$$
 (22)

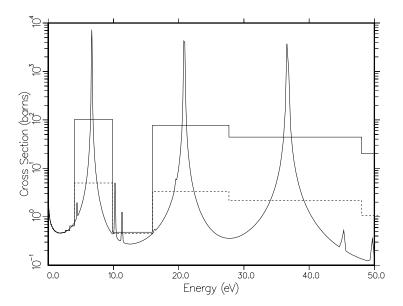
#### G. Self-Shielding

Eq. (1) is a multigroup approximation to the Boltzmann equation, and the energy texture is necessarily coarse with respect to the resonance structure in

## MULTIPARTICLE COUPLED SET



**Figure 2:** Layout of a coupled table for the simultaneous transport of neutrons, protons, and gamma rays. Normally, only the lower triangle of the "p to n" block would contain values for the upscatter portion of the table (the part above the line in the middle). The "group" index increases from left to right, and the "position" index increases from top to bottom.



**Figure 3:** Comparison of pointwise and multigroup representations of <sup>238</sup>U capture. The solid histogram shows the effective multigroup cross sections for infinite dilution, and the dashed histogram shows the effective cross sections for a background cross section of 30 barns/atom. This is the 69-group structure used in the MATXS7 library.

many materials. Fig. 3 compares the pointwise and groupwise representations of the first three capture resonances of  $^{238}$ U. A resonance material in a dilute mixture or in small pieces does not disturb a smooth flux very much by its presence—this is called the infinitely dilute case—but more resonance material will cause sharp dips in the flux corresponding to each resonance. The reaction rate  $\sigma\phi$  will be reduced. The resonance is said to be "self-shielded."

The magnitude of this self-shielding effect is in general a complicated function of the geometry and composition of the system. However, it has been found that a simple model called the Bondarenko Method<sup>16</sup> or Background Cross Section Method<sup>17</sup> does a surprisingly good job of representing the effects for many applications. The flux is assumed to vary inversly as the total macroscopic cross section. The model flux for the group averages for isotope i is written as

$$\phi_{\ell}^{i}(E) = \frac{C(E)}{[\sigma_{0}^{i} + \sigma_{\ell}^{i}(E)]^{l+1}} \quad , \tag{23}$$

where C(E) is the smooth part of the shape of the flux, and  $\sigma_0^i$  is called the background cross section (it represents the effects of all the other isotopes). The effect of the total cross section in the denominator is to put a dip in the flux

for each peak in the cross section, and  $\sigma_0^i$  controls the relative size of the dip  $(\sigma_0^i = \infty \text{ gives the infinitely dilute case discussed above})$ . The  $\ell$  dependence shown here is appropriate for a large system with nearly isotropic scattering (*i.e.*, the  $B_0$  approximation), and it was used when the MATXS files were generated. The result in Eq. (23) is based on the narrow resonance approximation, and it will be less accurate for some of the wider low-energy resonances important in thermal systems. The multigroup form of this model flux is

$$\phi_{\ell g}^{i} = \frac{C_g}{[\sigma_{0g}^{i} + \sigma_{tg}^{i}]^{l+1}} \quad . \tag{24}$$

For an infinite homogeneous mixture, the appropriate background cross section is

$$\sigma_{0g}^i = \frac{1}{N_i} \sum_{j \neq i} N_j \, \sigma_{tg}^j(\sigma_{0g}^j) \quad , \tag{25}$$

where  $N_i$  is the number density for the isotope. Because  $\sigma_t$  depends on  $\sigma_0$ , finding  $\sigma_0$  is clearly an iterative process.

For a lump of resonance material embedded in a large moderating region, escapes from the lump also increase the background cross section. This additional escape cross section is given by

$$\sigma_{xg}^i = \frac{1}{N_i \overline{\ell}} \quad , \tag{26}$$

where  $\overline{\ell}$  is the mean chord length of the lump given by

$$\overline{\ell} = \frac{4V}{S} \quad , \tag{27}$$

and where V and S are the volume and surface area of the lump (e.g., for a cylinder,  $\overline{\ell}=2r$ ). The mean chord  $\overline{\ell}$  can be adjusted away from the geometric value of Eq. (27) to compensate for the presence of other lumps (Dancoff corrections) or for shortcoming in the escape probability model used to obtain Eq. (26) (Bell factors); the main point is that TRANSX option provides an additional component for the background cross section that is parameterized by  $\overline{\ell}$ .

Eqs. (25) and (26) show that there is some kind of equivalence between the self-shielding effects of an admixed moderator and the self-shielding effects of heterogeneity. Physically, in the narrow-resonance regime, if a neutron is produced at the energy of an absorption resonance of material i, either losing energy by scattering from one of the competing materials j or escaping from the lump will assure

that it will not be absorbed by that resonance. In fact, the effects are additive. As an example, consider a 1-cm rod of uranium oxide surrounded by a large region of moderator:

$$\sigma_0 = \frac{.046 \text{ at/b-cm} \times 3.76 \text{ b/at}}{.023 \text{ at/b-cm}} + \frac{1 \text{ cm}}{.023 \text{ at/b-cm}}$$

$$= 7.52 \text{ b/at} + 43.48 \text{ b/at}$$

$$= 51.0 \text{ b/at}$$

where .023 and .046 are the atomic densities of the <sup>238</sup>U and oxygen, respectively, and 3.76 barns is the oxygen cross section.

#### H. Dancoff Corrections

If the lumps, rods, or plates containing the resonance material are arranged in a lattice or stack, it is likely that a neutron starting from one lump could pass through the matrix material and react with the fuel in another lump. Such an event is equivalent to never having escaped from the first lump at all; therefore, the escape cross section is reduced. This is called a Dancoff correction, and several options are available in TRANSX:

Cylinder by the Bell approximation,

$$C = \frac{1}{1+\lambda} \quad ; \tag{28}$$

Cylinder in an hexagonal lattice by the Sauer approximation,

$$C = \frac{e^{-\tau\lambda}}{1 + (1 - \tau)\lambda} \quad ; \tag{29}$$

where

$$\tau = \left(.9523\sqrt{1 + \frac{V_M}{V_M + V_C}} - 1\right) \frac{\sqrt{1 + V_C}}{V_M} - .12\left(1 + \frac{1}{2}\sqrt{\frac{V_C}{1 + V_C}}\right) \quad , \tag{30}$$

Cylinder in a square lattice by the Sauer approximation,

$$C = \frac{e^{-\tau\lambda}}{1 + (1 - \tau)\lambda} \quad ; \tag{31}$$

where

$$\tau = \left(.8862\sqrt{1 + \frac{V_M}{V_M + V_C}} - 1\right) \frac{\sqrt{1 + V_C}}{V_M} - .08\left(1 + \frac{1}{2}\sqrt{\frac{V_C}{1 + V_C}}\right) \quad , \tag{32}$$

Slab cell by the Bell approximation,

$$C = \frac{0.5}{1 + \lambda_B} + \frac{0.5}{1 + \lambda_L} \quad ; \tag{33}$$

and

Slab cell by  $E_3$  collision probabilities,

$$C = E_3(\lambda_R) + E_3(\lambda_L) . (34)$$

In these expressions,  $\lambda$  stands for the optical path in the moderator region,  $\overline{\ell}_m \sigma_m$ ,  $\lambda_L$  and  $\lambda_R$  are the optical paths to the left and right from the region containing material i to the next slab containing the same material,  $V_M$  and  $V_C$  are the ratios of the moderator volume and clad volume to the fuel volume, and  $E_3$  is the third-order elliptic integral. In all the cases, the Dancoff correction results in an escape cross section of

$$\sigma_{xg}^{i} = \frac{1}{N_{i}\overline{\ell}} \frac{b_{1}(1-C)}{1+(b_{2}-1)C} , \qquad (35)$$

where  $b_1$  and  $b_2$  are called Bell corrections (appropriate values are 1.09 for slabs and 1.35 for cylinders). When  $b_1=b_2$ , the constant is usually called A, the Levine factor. TRANSX provides for the automatic calculation of fuel and moderator mean chords and homogenized moderator cross sections, given the volumes and compositions of the various regions of a cell. Examples are given later in this report.

#### I. Interpolation in Cross Section Tables

The self-shielded cross sections for the MATXS libraries are computed in the GROUPR module of the NJOY system using Eqs. (3) and (4) together with the flux model of Eq. (23) and, optionally, using the flux calculator, for a preselected set of temperatures and background cross sections  $\sigma_0$ . To obtain a cross section at some other temperature and background cross section, it is necessary to interpolate between the values in the library.

The variations of the cross sections with temperature are normally fairly simple. Earlier versions of TRANSX used a N-th order Lagrangian interpolation scheme on  $\sigma(T)$  and T, where T is the temperature and N is the number of values in the temperature grid. However, this scheme would sometimes give unphysical or negative cross sections due to oscillations in the interpolation function. This version of TRANSX reverts to using simple linear interpolation for its stability.

For  $\sigma_0$ , the shielding curve has a shape similar to the tanh function (see Kidman). <sup>18</sup> Like tanh, it has a limited radius of convergence, and no single polynomial can be used to represent it for all  $\sigma_0$ . Earlier versions of TRANSX used a combination of  $1/\sigma_0$ , Lagrangian, and quadratic interpolation for different  $\sigma_0$  ranges. Just as for temperature interpolation, this scheme sometimes led to large unphysical oscillations in the interpolated cross sections. Therefore, this version of TRANSX uses simple linear interpolation based on  $\log(\sigma_0)$ , except for very large  $\sigma_0$  values, where it uses  $1/\sigma_0$  interpolation. The lowest cross-section value is used for  $\sigma_0$  less than the lowest grid point in the self-shielding table. This approach is stable and reliable, but it requires that data be given on a finer  $\sigma_0$  grid than the older method for equivalent accuracy. Note also that linear interpolation preserves the condition that the total cross section be equal to the sum of its parts.

## J. Elastic Scattering Corrections

In order to make a library of multigroup constants, as defined by Eqs. (3) and (4), it is necessary to choose a model-weighting flux. In an actual system, the real flux may be quite different from this model. Because the flux will usually vary from region to region, the mismatch between the actual and model flux cannot always be removed by improving the library flux. For the vector cross sections (e.g., capture, fission), the size of a group can usually be made small enough so that the weighting flux difference is not too important. However, the elastic downscatter for the heavier materials always takes place from a range of energies very close to the bottom of the group. If r is the ratio of the flux near the botton of a group to the group-average flux, the elastic removal cross section is very sensitive to any difference between r calculated for the actual flux and r calculated for the model flux.

Starting with the 1DX code, <sup>19</sup> various attempts have been made <sup>20</sup>, <sup>21</sup> to correct the elastic removal based on the shape of the computed flux using an iterative scheme. However, the complicated consequences of resonances in the cross sections make this dangerous except in regions where the calculated flux varies smoothly. Therefore, TRANSX does not attempt to correct for variations that only show up

in one or two groups. Instead it smoothes the flux by averaging over several groups above and below the group in question. This results in an effective slope for the flux near the bottom of the group, which can be used to correct the removal as shown below. The corrected cross-section set should give improved answers for any responses that depend on the average removal effect such as  $k_{\rm eff}$ , but the actual flux shape near a particular resonance may not be improved at all.

The removal from group q to group q' can be written

$$R_{g'\leftarrow g}^{M} = \int_{g} du \int_{g'} du' \sigma_{e}(u'\leftarrow u) \phi^{M}(u) , \qquad (36)$$

where u is lethargy,  $\sigma_e$  is the elastic scattering differential cross section, and  $\phi^M$  is the model flux. If the actual flux at the bottom of the group has a different slope than the model flux,

$$\phi(u) = [a - b(u_g - u)]\phi^M(u) \quad , \tag{37}$$

where  $u_g$  is the lethargy at the bottom of group g, the removal rate becomes

$$R_{g' \leftarrow g} = R_{g' \leftarrow g} [a - b\gamma_{g' \leftarrow g}] \quad , \tag{38}$$

where

$$\gamma_{g' \leftarrow g} = \frac{\int_{g} du \int_{g'} du' (u_g - u) \, \sigma_e(u' \leftarrow u) \, \phi^M(u)}{\int_{g} du \int_{g'} du' \, \sigma_e(u' \leftarrow u) \, \phi^M(u)} \quad . \tag{39}$$

The quantity  $\gamma_g = \sum_g \gamma_{g' \leftarrow g}$  is available on the MATXS library, so this  $\gamma$  is used for all groups and Legendre orders to obtain the corrections to the elastic scattering matrix elements.

It is then assumed that the smoothed flux ratio can be represented by

$$\ln(\phi/\phi^M) = x_0 + x_1(u_g - u) + x_2(u_g - u)^2 , \qquad (40)$$

in the group g. The coefficients are computed using a least squares fit to six values of the ratio assigned to the lethargy center of each of the six groups (three above  $u_g$  and three below). The parameters a and b are determined at the bottom of the group, and the smoothed value of the ratio at the center of the group is used to find the change in cross section that will give the desired change in removal rate.

The method is very stable. It avoids the divergences in removal cross sections often seen with other methods, and it usually converges adequately in one iteration.

## K. Group Collapse

It is necessary to produce cross-section libraries with fairly narrow energy groups to minimize the consequences of an inappropriate model flux discussed above. However, it may not be economical (or even possible) to perform a multi-dimensional  $S_N$  solution using the fine-group structure directly. In such cases it is desirable to collapse to a coarser group structure. The collapse can be defined in such a way as to preserve each term of the  $P_N$  equations when they are summed over all fine groups g in coarse group G as follows:

## Coarse group flux

$$\phi_{\ell G} = \sum_{g \in G} \phi_{\ell g} \quad , \tag{41}$$

Absorption,  $\bar{\nu}\sigma_f$ , and edit cross sections

$$\sigma_{xG} = \sum_{g \in G} \sigma_{xg} \frac{\phi_{0g}}{\phi_{0G}} \quad , \tag{42}$$

Transport cross section for leakage calculation

$$\sigma_{trG}^{PN} = \sum_{g \in G} \sigma_{trg}^{PN} \frac{\phi_{1g}}{\phi_{1G}} , \qquad (43)$$

 $P_{\ell}$ -weighted total cross section

$$\sigma_{\ell tG}^{PN} = \sum_{g \in G} \sigma_{\ell tg}^{PN} \frac{\phi_{\ell g}}{\phi_{\ell G}} \quad , \tag{44}$$

Scattering matrix cross sections

$$\sigma_{\ell G \leftarrow G'}^{PN} = \sum_{g \in G} \sum_{g' \in G'} \sigma_{\ell g' \leftarrow g}^{PN} \frac{\phi_{\ell g'}}{\phi_{\ell G'}} , \qquad (45)$$

and

Steady-state and delay fission spectrum  $\chi$ 

$$\chi_G = \sum_{g \in G} \chi_g \quad . \tag{46}$$

The coarse-group  $S_N$  equations can be derived from the coarse-group  $P_N$  equations; therefore, Eqs. (7) through (13) apply with g replaced by G.

The flux components can be read in from some previous calculation or generated from the model weight function used to generate the MATXS library with

$$\phi_{\ell g} = \frac{C_g}{\prod_{k=0}^{\ell} [\sigma_{0q} + \sigma_{ktq}]} . \tag{47}$$

In practice only k=0 and k=1 are available on the MATXS library, and k=1 is used for all higher orders.

Note that there are four different uses for input fluxes in TRANSX: (1) collapse, (2) fission  $\chi$ , (3) transport cross section and (4) elastic scattering corrections.

## L. Spatial Collapse

It is often necessary to replace the complex geometry of a reactor cell with some effective average cross section before doing two- or three-dimensional calculations for an entire reactor core. This spatial collapse is similar to the group collapse described above in that both try to preserve the terms of the  $P_N$  equation. Using  $v_i$  for the region volumes and V for the cell volume gives the following results:

#### Cell-average flux

$$\phi_{\ell g}(V) = \sum_{i \in \text{cell}} \frac{\phi_{\ell g}(v_i) \, v_i}{V} \quad , \tag{48}$$

and

Cell-average macroscopic cross section

$$\Sigma_{\ell g}(V) = \sum_{i \in \text{cell}} \sum_{j} \frac{\rho_{j}(v_{i}) \,\sigma_{\ell g}^{j}(v_{i}) \,\phi_{\ell g}(v_{i}) \,v_{i}}{\phi_{\ell g}(V) \,V} \quad . \tag{49}$$

In these equations, the  $v_i$  are the region volumes, V is the cell volume,  $\rho_j(v_i)$  is the number density for material j in region i, and  $\sigma_{\ell g}^j(v_i)$  is the microscopic cross section for material j in region i.

These calculations of cell-averaged quantities require a good knowledge of the region fluxes by group. These fluxes can be obtained in the form of a CCCC standard-interface file from a separate transport calculation and read into TRANSX. A typical procedure is to do a simple one-dimensional calculation for

a reactor pin cell, and then to use the flux from this calculation to prepare cellaveraged cross sections to be used for a reactor-core calculation. An example of this process will be found in the next section of this report.

It is often necessary to obtain a "constituent" of a mixture like this, for example, the microscopic cross section for the <sup>235</sup>U in the uranium oxide in the fuel region of a reactor pin. Other times, the user may need the microscopic cross section averaged over the cell. TRANSX calls the first type of constituent cross section a "region constituent" and the second type a "cell constituent."

Region constituents are useful when the transport calculation is going to be done using the detailed region-wise geometry of the cell and when the user needs to make the mixtures in the transport code (e.g., to do concentration searches). Real material densities must be used with region constituents.

Cell constituents include the effects of any flux depression ("disadvantage factors") or flux enhancement in the regions of the cell. Therefore, they are needed when the transport calculation is going to be made using a simplified geometry and when the user needs to make the mixtures in the transport code. Cell-averaged densities must be used with cell constituents.

## M. Photon Production Self-Shielding

Photons are produced by capture and fission, and both reactions usually show significant self-shielding in resonance energy ranges. Although the MATXS format has the capability of storing shielded cross sections for any photon production cross section, the current libraries contain only infinite-dilution photon matrices, and TRANSX uses shielding factors for the corresponding neutron reaction to self-shield each photon production matrix.

## N. Thermal Cross Sections

When the energy of a neutron is comparable with the energy of thermal motion of the atoms in a material, the neutron can gain energy in a collision, or "upscatter." Most  $S_N$  codes can handle upscatter at some increase in run time. The location of the upscatter groups in the transport table is defined in Table 1.

The detailed thermal cross sections and scattering matrices depend upon the binding between the atoms of the material. Therefore, MATXS thermal libraries will contain several sets for a particular isotope, for example, H in  $H_2O$ , H in polyethylene, and H in ZrH. In addition, thermal scattering can have both coherent and incoherent components. Coherent scattering takes place with no energy change

(in-group only) and includes the diffraction effects of the neutron wave interacting with the entire crystalline lattice. The incoherent part contains both energy-gain and energy-loss cross sections due to interactions with lattice vibrations or molecular rotation and vibration modes. For the heavier materials, it is often a good approximation to treat the atoms as a gas of free particles at the appropriate temperature. Free-gas cross sections and matrices are included on MATXS thermal files for all materials in addition to any bound cross sections given for important moderator materials.

Thermal cross sections are defined over a limited energy range (e.g., E<4 eV). To prepare an upscatter set, TRANSX corrects the total cross section by subtracting the normal static elastic cross section (NELAS) and adding back the appropriate incoherent and coherent thermal cross sections over the requested energy range. This step ensures that any absorption reactions are included. For the scattering matrix, TRANSX uses the static matrix above the specified energy range and the requested incoherent and coherent matrices below the energy cutoff. Sources from above the cutoff to below use elements of the static matrix. Sources from below the cutoff to above are truncated into the last group of the thermal range so that there is no upscatter for groups above the cutoff.

Some ENDF/B thermal evaluations give the scattering from each atom in the molecule, and the different atoms must be combined in TRANSX. An example is water; here "H in H<sub>2</sub>O" must be combined with free-gas oxygen. Other evaluations (e.g., methane) give the entire scattering for the molecule with the principal scatterer (everything is renormalized to the cross section of the principal scatterer). In these cases, TRANSX must mix in the thermal scattering for the principal scatterer and omit the contribution for the secondary atom. Methods for doing this are discussed in the next section.

#### O. Epithermal Self-Shielding

The biggest weakness of the TRANSX code as described so far occurs for thermal reactor analysis in the "epithermal" energy region from about 4 eV to around 200 or 300 eV. In this region, the resonances are no longer "narrow," and the flux shape given by Eq. (23) is no longer sufficiently accurate. This failure is normally only important for resonance materials that are present in large concentration, such as  $^{238}$ U. TRANSX results for this energy range can be improved by preparing special cross sections for the  $^{238}$ U using the NJOY flux calculator. As an example, you could prepare a new isotope called U238B with cross sections appropriate for  $^{238}$ UO<sub>2</sub> in pins of a certain size surrounded by a

water region. You could then add this isotope to your MATXS library using BBC. By asking for U238B instead of U238 in your TRANSX run, you would get improved results for resonance self-shielding in the epithermal region.

#### III. HOW TO RUN TRANSX

TRANSX is capable of solving complex problems, and the input is necessarily complex. However, an attempt has been made to simplify the input by providing defaults so that the user interested only in the simpler problems can ignore some of the complexities. This section is organized from the simple to the complex; a user can stop reading when he knows enough to solve his problem.

The input instructions are given in the following subsection. They are explained in the subsequent subsections by using examples. The examples also act as test problems for the code, and some partial listings are included in Appendix A. Input decks and full output listings for all of these sample problems are included in the TRANSX 2.0 distribution package.

## A. TRANSX Input Instructions

The following user input instructions for TRANSX were copied from the comment cards at the beginning of the TRANSX source deck. It is always a good idea to check these cards in the current version of the code, because they are more current than the version printed here.

```
---USER INPUT (FREE FORM)-----
  CARD 1
          RUN TITLE (HOLLERITH DESCRIPTIVE COMMENT)
             72 CHARS MAX. NO DELIMITERS OR TERMINATOR REQUIRED.
             STOP TERMINATES JOB
  CARD 2
          OPTIONS
  IPRINT
           PRINT (O=LONG/1=SHORT)
  IOUT
           OUTPUT FORMAT
                NONE
             O
             1
                CARD (6E12)
             2
                CLAW (CARD WITH SEPARATE EDITS)
             3
                FIDO
             4
                 ANISN (FIDO WITH 2*L+1 FACTOR)
                GOXS (GROUP-ORDERED BINARY)
                 ISOTXS (CCCC-IV MATERIAL-ORDERED BINARY)
  IPROB
           PROBLEM (O=DIRECT/1=ADJOINT)
   ISET
           ISET=I FOR A SIMPLE SET FOR PARTICLE I,
           ISET=IJ FOR A COUPLED SET FOR PARTICLES I AND J,
           ISET=IJK FOR A THREE-WAY COUPLED SET, ETC.
  IFORM
           FORM (1=MATWISE/2=GROUPWISE)
           FISSION TIME (1=STEADY-STATE/2=PROMPT)
   ITIME
           DECAY TIME (RESERVED)
  IDECAY
  ITRC
           TRANSPORT CORRECTION
                NONE (NOT FOR SN CODES)
                CONSISTENT-P
             1
                DIAGONAL
```

- 3 BELL-HANSEN-SANDMEIER
- 4 INFLOW
- 5 INCONSISTENT-P

ICOLL COLLAPSE (O=NO/NFINE=YES)

INITF INITIAL FLUX

- O USE LIBRARY WEIGHT FOR PO FLUX
- 1 READ PO FLUX ON CARDS
- 2 READ RTFLUX INTERFACE (CCCC-IV TOTAL FLUX)
- 3 READ RZMFLX INTERFACE (ZONE MOMENTS FLUX)
- 4 READ RZFLUX INTERFACE (CCCC-IV ZONE FLUX)

12-14 TRIGGERS REMAP OF INPUT FLUX

-N MAKE ELASTIC SCATTERING FLUX CORRECTION (FOR LAST FIVE ITEMS, DEFAULT=FIRST OPTION)

CARD 3 PARAMETERS

NGROUP NUMBER OF GROUPS IN TABLE NL NUMBER OF LEGENDRE TABLES

NTABL TABLE LENGTH

NUP NUMBER OF UPSCATTER GROUPS NTHG NUMBER OF THERMAL GROUPS

NMIX NUMBER OF OUTPUT MIXES OR MATERIALS

NREG NUMBER OF REGIONS

NMIXS NUMBER OF MIX SPECIFICATIONS

NED NUMBER OF EXTRA EDITS

NEDS NUMBER OF EDIT SPECIFICATIONS

CARD 4 MIX NAMES

HMIXN NMIX HOLLERITH MIX NAMES (6 CHARACTERS MAX)

CARD 5 REGION AND HETEROGENEITY SPECS

HREGN REGION HOLLERITH NAME (6 CHARACTERS MAXIMUM)

RTEMP REGION TEMPERATURE (K) (DEFAULT=300)

RVOL REGION VOLUME (DEFAULT=1.)

IHET HETEROGENEITY OPTION (DEFAULT=0=NO SELF SHIELDING)

- O NO SELF SHIELDING
- 1 CONSTANT ESCAPE CROSS SECTION
- 2 CYLINDER BY BELL APPROXIMATION
- 3 CYLINDER IN HEX LATTICE BY SAUER APPROXIMATION
- 4 CYLINDER IN SQUARE LATTICE BY SAUER APPROXIMATION
- 5 SLAB CELL BY BELL APPROXIMATION (REFLECTIVE)
- 6 SLAB CELL BY E3 APPROXIMATION (REFLECTIVE)
- 7 SLAB CELL BY BELL APPROXIMATION (PERIODIC)
- 8 SLAB CELL BY E3 APPROXIMATION (PERIODIC)
- -N CONTINUE SPECIFYING THE CELL

THE REST OF THE PARAMETERS ON CARD 5
DEPEND ON THE VALUE OF IHET. THESE VALUES
ARE ONLY GIVEN FOR THE FIRST REGION OF EACH CELL.

-- IHET=1 -- CONSTANT ESCAPE

CHORD MEAN CHORD LENGTH (CM)

#### -- IHET=2 THRU 8 -- DANCOFF APPROXIMATIONS

BELL1 BELL CORRECTION TO RATIONAL APPROX.

BELL2 BELL CORRECTION TO DENOMINATOR

#### REPEAT CARD 5 NREG TIMES

CARD 6 REMAP INSTRUCTIONS (ABS(INITF).GE.12 ONLY)
FLUX POINT, ZONE, OR REGION FROM INPUT FILE TO BE
ASSIGNED TO EACH TRANSX REGION (NREG INTEGERS)

CARD 7 MIX SPECIFICATIONS

IMIX MIX NUMBER (O TO NMIX)

IREG REGION NUMBER

HMIX NAME OF ISOTOPE FROM MATXS

DENS MULTIPLIER (FRACTION OR DENSITY) (DEFAULT=1)

HINC THERMAL INELASTIC NAME (DEFAULT=BLANK),

OR CONSTITUENT CROSS SECTION FLAG

("RC" FOR REGION CONSTITUENT, OR "CC" FOR CELL)

HCOH THERMAL ELASTIC NAME (DEFAULT=BLANK)

HMOD MATRIX MOD REACTION (DEFAULT=BLANK=TOTAL)

#### REPEAT CARD 7 NMIXS TIMES

CARD 8 EDIT NAMES

HED NED HOLLERITH EDIT NAMES (6 CHARACTER MAXIMUM)

CARD 9 EDIT SPECIFICATIONS

JEDPOS EDIT POSITION (USUALLY IN RANGE FROM 1 TO NED)

(-N TO PUT DELAYED GAMMAS IN GROUP N OF COUPLED SET)

HEDNAM NAME OF REACTION FROM MATXS

EDFACT MULTIPLIER (DEFAULT=1)

HEDMAT ISOTOPE NAME FROM MATXS (DEFAULT=BLANK)

IF BLANK, USE SPECIFICATION FOR ALL ISOTOPES

#### REPEAT CARD 9 NEDS TIMES

CARD 10 COLLAPSE SPECIFICATIONS (IF ICOLL.NE.O)
INPUT NUMBER OF FINE GROUPS IN EACH COARSE GROUP

CARD 11 INPUT FLUX FUNCTION (INITF=1 ONLY)

INWT FLUX FOR FINE GROUPS TO BE USED FOR

ALL ORDERS AND ALL REGIONS

#### SPECIAL INPUT VALUES

HED=\*CHI\* THIS POSITION TO CONTAIN FISSION CHI

HEDNAM=\*CHI\* DITTO

HED=\*TRD\* THIS POSITION TO CONTAIN TRANSPORT

CROSS SECTION FOR DIFFUSION. IF A P1 FLUX IS GIVEN OR COMPUTED, THE INFLO DEFINITION WILL BE USED. OTHERWISE, OUTFLO WILL BE USED.

HEDNAM=\*TRD\* DITTO

HED=\*GAM\* THIS POSITION TO CONTAIN THE FIRST OF NGG GAMMA

#### PRODUCTION EDITS

\*

### B. Free Form Input

All input to TRANSX is free form with no limitation to fixed fields. Numbers do not require decimal points, but the "E" is required when exponents are given. Hollerith strings are delimited with stars (\*) or preceded by "nH" as in FORTRAN formats. Delimiters are not necessary if the string is a single word (i.e., six or fewer characters) and starts with a letter. The construction "nR" causes the following entry to be repeated n times. Entries can be separated by any character not used for another purpose. A comma works, but spaces look better. Lines can be terminated early with /, and any input values not given are defaulted as defined in the input instructions. Any text appearing to the right of a / (other than a / embedded in a Hollerith string) will be treated as a comment. Lines beginning with a \$ sign will also be treated as comments. Care must be used to include the / when needed; otherwise, the input routine will keep on reading cards until it has found the requested number of entries or reaches the end of the file. The proper input syntax should be made clear by the examples below.

TRANSX input card 1 is not read by the free-format input processor; it is read by a simple FORTRAN statement. Therefore, stars are not required. The "stop" at the end of a TRANSX input deck is a special case of card 1, and stars are not required there either (although they can be given).

#### C. Simple Transport Tables

The following examples illustrate simple microscopic and macroscopic crosssection sets without self-shielding or thermal upscatter. Simple response edits, group ordering, and collapse are shown also.

Sample Problem 1. Simple Material-Ordered Tables

```
TEST 1 -- MATERIAL ORDERED TABLES
       1 1 1 0 3
      34 0 0 3 1 6 1 1
CARBON TUNGST U-235
     CNAT/
     W182 .263/
     W183
          .143/
2
     W184
          .307/
  1
     W186
          .286/
  1
  1
     U235/
```

HEAT

1 HEAT 1.602E-19/ CONVERTED TO JOULE-BARNS
STOP

The cross sections will be read from a file named MATXS (see Section V), and the neutron tables will be printed and written onto a file named CARD as 6E12 cards (see Section IV for a complete description of the interface files) in material ordering. Fission will be steady state, and the BHS transport correction will be used. Because two tables are requested ( $P_0$  and  $P_1$ ), the BHS correction will be derived from the P<sub>2</sub> data on the library. The table length of 34 is enough to accommodate all 30 groups, the three standard edits  $(\sigma_a, \bar{\nu}\sigma_f, \sigma_t)$ , and one special edit. There are no upscatter positions or thermal groups requested. Three output materials are defined with the names given. Note that these names are independent of the isotopes on the library and will only be used to label the output and to name the materials on the output file CARD. The materials lie in a region with temperature 300 K (by default) and a blank name, but "region" has no other significance here in the absence of an input flux or self-shielding. The six mix instructions use default values for simplicity. This table works as follows: The material HMIX is multiplied by DENS (default=1.) and added into mixture IMIX. The names used for HMIX must correspond exactly to material names on the MATXS library. The use of atom fractions for DENS in mix 2 produces the correct microscopic cross sections for natural tungsten. Later examples will show how to generate mixed macroscopic cross sections. The response edit "HEAT" is intended to give nuclear heating in watts/cm<sup>3</sup> when folded with a flux in a transport code. The table works just like the mix table. The cross section HEDNAM from the MATXS library is multiplied by EDFACT and added into position JEDPOS. The EDFACT shown here converts KERMA factors from eV-barns to Joule-barns. Just as for material names, the reaction names (e.q., HEAT) for HEDNAM must correspond to names on the library, but the edit name (e.g., HEAT) is only used for labeling the output. The last card is read as the title for the next case, but "STOP" has the special meaning of ending the run. The meaning of these input parameters may be clarified by the partial listings of the OUTPUT and CARD files in Appendix A.

### Sample Problem 2. Group Ordering

This is the same as Problem 1 except for group-ordered printed output. No library is written because no card image format is available for IFORM=2. See Appendix A.

## Sample Problem 3. Coupled Set

```
TEST 3 -- COUPLED SET

0 3 0 3 1 1 0 3 0 0

42 2 46 0 0 1 1 2 1 2

AL-27

* */
1 1 AL27/

HEAT

1 HEAT/ NN AND NG PART

1 GHEAT/ GG PART

STOP
```

This time output in FIDO format was requested. As described in Section IV-E, FIDO suppresses many of the zeroes in the output file. The coupled option was selected, and 42 had to be given for the number of groups (MATXS5 is a 30 x 12 library). The nn, ng, and gg blocks for AL27 are automatically moved to the correct part of the coupled set. The photoatomic data are really elemental in nature, but the MATXS file now contains duplicate tables for each isotope, for convenience, and it is no longer necessary to name both AL27 and AL in TRANSX input decks. The edit cross sections GHEAT and HEAT are also automatically moved to their proper positions in the coupled set; the former ends up as position 1 for groups 31 to 42, the latter in groups 1 to 30. A partial listing of the FIDO tables is given in Appendix A.

## Sample Problem 4. Cross Sections for GODIVA

```
TEST 4 -- GODIVA
0 1 0 1 1 1 0 3 30 1
20 4 34 0 0 1 1 3 1 0
CORE
CORE/
    U235 .0450/
1 1
1 1
     U238
          .002498/
1 1
     U234 .000492/
CHI
19R1 11/ COLLAPSE OUT BOTTOM 11 GROUPS
6.80E-8 1.72E-7 5.78E-7 3.30E-6 1.88E-5 5.92E-5 3.52E-4 3.21E-4
4.00E-4 4.43E-4 4.61E-4 8.79E-4 7.74E-4 5.90E-4 3.53E-4 2.83E-4
6.30E-5 9.77E-6 1.27E-6 1.62E-7 1.87E-8 2.23E-9 3.41E-10 3.56E-11
5.38E-12 2.29E-12 9.15E-13 1.30E-15 7.63E-19 1.59E-22/
STOP
```

GODIVA is a bare sphere of enriched uranium that is often used as a cross-section benchmark.<sup>23</sup> In this example, macroscopic  $P_3$  cross sections are produced directly. As a result, it is not necessary to mix cross sections in the transport code. In addition to saving time and storage space, this approach allows a mixture-dependent

fission  $\chi$  to be formed. Because the spectrum of GODIVA is rather hard, the lower energy groups are collapsed down to fewer groups (note the use of the repeat specification). An initial flux guess is read in from the input file to improve the estimate for the fission spectrum  $\chi$  and to improve the group collapse. Note that ICOL=30, the number of fine groups, and NGROUP=20, the number of coarse groups for the output material. CHI is a special edit command that does not require any further specification.

## D. Advanced Response-Function Edits

One of the powers of TRANSX is its ability to produce varied response-function edit cross sections. The ability arises partly out of TRANSX, which can produce any edit that is a linear combination of any cross sections on the MATXS file, and partly out of MATXS, which contains all of the partial cross sections available in the original ENDF/B evaluations as well as some additional quantities, such as nuclear heating and radiation damage cross sections.

As an example of the power of linear combination, consider the problem of computing the helium production rate in graphite. The  $^{12}$ C evaluation in ENDF/B-IV includes an  $(n, \alpha)$  reaction (called NA) and a continuum  $(n, n')3\alpha$  reaction (NCNAAA). An edit for helium production rate (arbitrarily named N.HE4) can be obtained using the following edit specifications:

```
...
N.HE4
1 NA/
1 NCNAAA 3./
```

The NA reaction is multiplied by 1 (default) and added into position 1, and the NCNAAA reaction is multiplied by 3 and added into position 1. Caution: A different representation is used in ENDF/B-V and VI.

Sometimes it is useful to define special edits for particular materials. As an example, the ratios of <sup>235</sup>U capture to <sup>235</sup>U fission and <sup>238</sup>U fission to <sup>235</sup>U fission were measured at the center of the GODIVA critical assembly. <sup>23</sup> The following edit specifications added to Problem 4 will provide the responses needed to compute these reaction rate ratios:

```
CHI F25 F28 C25
2 NFTOT 1. U235
3 NFTOT 1. U238
4 NG 1. U235
```

Note that the standard transport tables reserve NED words for each group, order, and material for edits that are not required during the flux calculation but only at the end of the problem when responses are computed. Also, the edits only appear in the  $P_0$  table, so the words reserved in the higher tables are wasted. Storage requirements can be reduced by defining a special edit table with NTABL=NED, which is only read during the response function edit calculation in the  $S_N$  code. The ONEDANT<sup>4</sup> code uses this approach.

## Sample Problem 5. Detailed Edit Table

```
TEST 5 -- EDIT TABLE
0 5 0 1 2 1 0
                     0
                        0 0
30 1 13 0 0 1 1 1 13 37
AL-27
AL-27/
1 1
     AL27/
ELAS NNG N2N
                N3N NG
                         NΑ
   ND NT NNP
                 NNA
N.1H N.4HE
  NELAS/
2
  NINEL/
2
  N75P
         -1/
  N78P
         -1/
2
  N80P
         -1/
2
  N81P
2
  N82A
        -1/
   N83P
         -1/
2
  N84P
         -1/
2
  N85P
         -1/
2
  N86A
         -1/
3
  N2N/
4
  N3N/
5
  NG/
6
  NA/
7
  NP/
8
  ND/
  NT/
9
10
   N75P/
   N78P/
10
   N80P/
10
10
   N81P/
   N83P/
10
10
   N84P/
10
   N85P/
   N82A/
11
   N86A/
11
12
   NP/
12
   N75P/
   N78P/
12
12
   N80P/
   N83P/
12
```

```
12 N84P/
12 N85P/
13 NA/
13 N82A/
13 N86A/
STOP
```

The <sup>27</sup>Al evaluation includes some discrete-inelastic levels that decay by proton or alpha emission rather than by a cascade of photons. The cross-sections for these reactions are subtracted from the total inelastic cross section in position 2 to obtain an isolated  $(n, n')\gamma$  reaction. The parts that were subtracted are added back into positions 10 and 11 to obtain (n, n'p) and  $(n, n'\alpha)$ , respectively. They are also added to the (n, p) and  $(n, \alpha)$  reactions in positions 12 and 13 to obtain the gas production cross sections for <sup>1</sup>H and <sup>4</sup>He, respectively.

Note that the detailed aluminum edits are written into a group-ordered binary interface file with the name GOXS (see Section IV-H). If its name is switched to SNXEDT, the ONEDANT edit module can read the file directly.

An important mechanism of radiation damage in metals is the displacement of atoms from their normal lattice positions caused by the recoil particle of a nuclear reaction. The energy available for producing displacements is given on the MATXS file as the damage energy production cross section DAME in eV-barns; it is less than the primary recoil energy because some of the energy causes electronic excitations rather than displacements. The primary recoil atom loses some of its energy ejecting another atom, giving a pair of displacements; each of these generates another pair, and so on, until all the energy is used up. The number of displacements produced by this cascade is equal to the damage energy divided by twice the energy required to displace one atom from its normal site. Various values of the displacement energy are used in practice; some values <sup>24</sup> are given in Table 2, which can be used to determine the EDFACT needed to convert the damage edit DAME into a "Displacement Per Atom" (DPA) edit. The use of this factor is illustrated below.

Except for the delayed neutron parameters CHID and NUD, all the other data on the current MATXS files are prompt data. However, many reactions such as

$$n + {}^{7}\text{Li} \rightarrow {}^{8}\text{Li} \rightarrow \beta^{-} + 2\alpha \quad (850 \text{ ms})$$

and

$$n + {}^{27}\mathrm{Al} \rightarrow {}^{28}\mathrm{Al} \rightarrow {}^{28}\mathrm{Si} + \beta^- + \gamma \quad (2.24 \text{ m})$$

Material	Energy (eV)	Material	Energy (eV)
Be	31	Fe	40
$\mathbf{C}$	31	Co	40
Na	25	Ni	40
Mg	25	Cu	40
Al	27	Zr	40
Si	25	Nb	40
K	40	Mo	60
Ca	40	Ag	60
Ti	40	Ta	90
V	40	W	90
$\operatorname{Cr}$	40	Au	30
Mn	40	Pb	25

**Table 2:** Typical values for the atomic displacement energy needed to compute DPA ( $\underline{D}$ isplacements  $\underline{P}$ er  $\underline{A}$ tom).

have decays that take place in times that are short with respect to the response desired. The steady-state heating due to capture in <sup>7</sup>Li should really be the sum of the prompt HEAT from the MATXS file and 9.31 MeV times the capture cross section. It can easily be produced with the following TRANSX edit specifications:

```
SSHEAT

1 HEAT/ PROMPT PART

1 NG 9.31E6/ DELAYED PART FROM 9.31 MEV CAPTURE GAMMA
```

The photon source from neutron reactions is also an interesting response that can be obtained with the special edit name GAM. Decay photons, such as the 1.779-MeV photon from the  $^{28}$ Al  $\beta^-$  decay mentioned above, can also be added into the photon source as shown in the next sample problem.

Sample Problem 6. Heat, Damage, and Photon Source

```
TEST 6 -- HEAT, DAMAGE, PHOTON SOURCE
0 1 0 1 1 1 0 3 0 0
30 2 47 0 0 1 1 1 14 4
AL-27
ALUM/
1 1 AL27/
HEAT DPA GAM GAM GAM GAM GAM
GAM GAM GAM GAM GAM
```

```
1 HEAT/
1 NG 1.125E6/
2 DAME .02/
11 NG/
STOP
```

The 12 occurrences of GAM reserve spaces for the 12 photon groups. Group 9 (1-2 MeV) is in position 11, and the last edit specification adds the equilibrium 1.779-MeV photon production rate into that group (one such delayed gamma is produced per capture event). Note also that damage energy is converted to DPA in position 2 using 25 eV for the displacement energy 0.02 = [1/(2\*25)]. Most  $S_N$  codes could use these cross sections and print out steady-state photon source vectors by region to be used in a subsequent photon transport calculation.

Coupled sets, like the one defined in Sample Problem 3, can also be prepared including steady-state radioactive decay contributions. Putting a negative sign on JEDPOS defines the gamma group in the coupled set that will receive the contributions defined by that edit specification. The Problem 3 input would become

```
TEST 3A -- COUPLED SET WITH STEADY-STATE DECAY
         3 1 1 0 3 0 0
      0
 42 2 46 0 0 1 1 2 1 2
 AL-27
 * */
 1 1
      AL27/
 HEAT
    HEAT/ NN AND NG PART
    GHEAT/ GG PART
 1
    NG
       1.125e6 AL27 / DELAYED HEAT AND GAMMAS FOR AL27
-8
   NG
       1.
                AL27
 1 NP
       3.2e5
                AL27
-10 NP
        .72
                AL27
-9 NP
                AL27
        .28
 STOP
```

Delayed heat and photon production edit specifications for some important materials are given in the DELAY12 and DELAY24 files included in the TRANSX distribution. As an example, the 12-group data for <sup>238</sup>U are repeated below:

```
1 N2N 0.060E+6 U238
   NG 0.160E+6
                  U238
   NF
        8.580E+6
                  U238
 1
    \mathtt{NF}
        5.995E-4
                  U238
-5
  NF
        4.072E-3
                  U238
    NF
        2.036E-2
                   U238
-7
    \mathtt{NF}
        9.226E-2
                  U238
-8
    NF
        3.033E-1
-9 NF 1.442E+0 U238
```

```
-10 NF 3.384E+0 U238
-11 NF 4.726E+0 U238
-12 NF 1.514E+0 U238
```

The heating part (position 1) includes the beta decay heating for <sup>239</sup>U and <sup>239</sup>Np; thus, it includes all the heat up to the appearance of the final <sup>239</sup>Pu product. The contributions to heating and photon production from fission come from the decay of the fission products.

## E. Self-Shielded Fast Reactor Problems

The simplest kind of self-shielding problem is one with simple homogeneous mixtures, for example, the one-dimensional model of the ZPR-6 assembly 7 critical assembly (see the ENDF benchmark descriptions).<sup>23</sup>

Sample Problem 7. ZPR-6/7 Spherical Homogeneous Model

```
TEST 7 -- ZPR-6/7 SPH. HOMOGENEOUS MODEL
     0 1 1 1 0 3 0
80 1 50 0 0 2 2 20 1 0
CORE BLANKET
CORE 300. 1. 1 10000/ HOMOGENEOUS SELFSHIELDING
                         HOMOGENEOUS SELFSHIELDING
BLANKT 300. 1. 1 10000/
     PU239 8.8672E-4/
     PU240
            1.1944E-4/
  1
     PU241 1.33E-5/
  1
     U235
             1.26E-5/
1
            5.78036E-3/
  1
     U238
1
  1
     MONAT 2.357E-4/
1
  1
     NA23
             9.2904E-3/
             .01398/
1
  1
     016u
     FE56
             1.297E-2/
1
            2.709E-3/
  1
     CR52
1
1
  1
     NI58
            1.240E-3/
1
  1
     MN55
             2.12E-4/
2
  2
     U235
             8.56E-5/
2
  2
     U238
             3.96179E-2/
     MONAT 3.8E-6/
2
  2
2
  2
     016
             2.4E-5/
2
  2
     FE56
            4.637E-3/
2
  2
             1.295E-3/
     CR52
2
  2
     NI58
            5.635E-4/
2
  2
            9.98E-5/
     MN55
CHI
STOP
```

The ENDF/B-VI libraries (which are used for all the test problems for TRANSX 2.0) contain the isotopes for iron, nickel, and chromium instead of the elemental

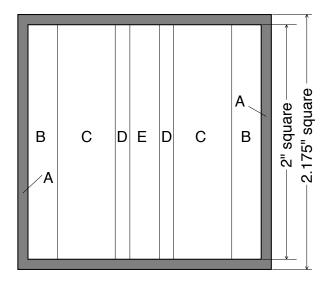
evaluations given in previous versions. The dominant isotope of each element has been used here to keep the problem input compact.

The cross sections are appropriate for diffusion theory or  $P_0$  transport theory. Note that the table length is less than the maximum 80+3+1. The scattering matrix is truncated in a way that preserves the scattering cross section (*i.e.*, down the diagonal). In this problem, there are two regions and two mixes. The mixes are macroscopic, and the fission  $\chi$  will be different in each region because the compositions are different. Self-shielding uses the constant-escape option with a temperature of 300 K. The region sizes are not needed for this problem, and they have been set to 1.0 for simplicity. The mean chord length for each region has been made very large (*i.e.*, no escape from the region) in order to obtain the mixture part of the self-shielding only. The background cross sections obtained are displayed on the printed output.

This homogeneous model is not completely adequate because the core and blanket regions are really made up of stacks of long slabs of the various materials arranged as repeating cells in a stainless-steel matrix. Figure 4 shows a simplified core cell. This heterogeneity has two effects; first, the background cross section for a material in a slab is changed because of the change in density and the addition of a slab escape probability; and second, the flux will be slightly different in each slab due to the sources and absorptions. The first effect is called heterogeneous self-shielding, and the second leads to the advantage and disadvantage factors for cell homogenization.

For the cell of Fig. 4, the self-shielding of  $^{239}$ Pu in E should be fairly well represented by the mixture effect in region E plus the escape cross section for a 0.5588-cm slab with a Dancoff correction corresponding to outside regions 4.965-cm thick ( $\bar{\ell}_{\rm m}=9.930$  cm) with the homogenized composition of A+B+C+D+clad on each side of the fuel slab. For the  $^{238}$ U in E, the outside regions extend only to B and would, therefore, be 1.626-cm thick with the C+D+clad composition on each side. The  $^{238}$ U in E sees different outside regions to the left (A+B+C+D+clad) and to the right (B+C+D+clad). The SS304 structures should be well represented by a 0.444-cm slab with outside regions with the A+B+C+D+E composition. Note that the mean chord would be only one-half of the infinite slab value, as  $\bar{\ell}_{\rm m}=5.08$  cm. These kinds of arguments can be completed for the other materials and regions in the cell.

This approach leads to separate two-region cell problems for each class of material (*i.e.*, all the plutonium isotopes in E from one two-region calculation, all the U isotopes in B from another), and TRANSX is capable of setting up the problem



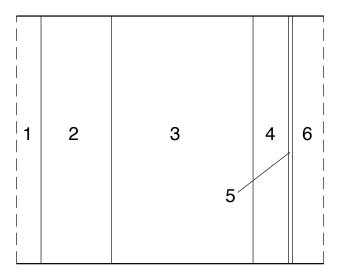
**Figure 4:** Simplified core unit cell for ZPR-6 Assembly 7. Region A is the SS304 structure (0.222 cm), B is a  $U_3O_8$  slab (0.635 cm), C is Na in an SS304 can (1.270 cm), D is an Fe<sub>2</sub>O<sub>3</sub> slab (0.3175 cm), and E is a Pu/U/Mo fuel slab in a can (0.635 cm). All can thicknesses are 0.0381 cm).

in this way. However, the result is very complex, and many dummy compositions are required.

A simpler representation is the multiregion slab cell shown in Fig. 5. This cell neglects the egg-crate SS304 structure and will overestimate the  $\sigma_0$  values for region 1. It also neglects the effect of the structure on any paths to regions 2 through 3; thus, there will be too much sodium and not enough iron. The resulting model is given in the following sample problem.

Sample Problem 8. ZPR-6/7 Sph. Heterogeneous Model

```
TEST 8 -- ZPR-6/7 SPH. HETERO MODEL
  3 0 1 1 1 0 3
                      0
           0 2 7 50 1
   2 50 0
CORE BLANKT
         .2223 6 2R1.09/
END
    300
U203
     300
         .6350 -6/
   300
       1.270 -6/
FE203
     300
          .3175 -6/
CLAD
     300
          .0381 -6/
          .2794
FUEL
     300
BLANKT/
     MONAT 5.0E-5/
            4.474E-2/
  1
     FE56
```



**Figure 5**: Approximate multiregion slab cell for ZPR-6 Assembly 7. The dashed lines represent reflection planes. Region 1 is the SS304 end slab (0.2223 cm), 2 is the  $U_3O_8$  slab (0.6350 cm), 3 is the sodium (1.270 cm), 4 is the Fe<sub>2</sub>O<sub>3</sub> slab (0.3175), 5 is the cladding (0.0381 cm), and 6 is the fuel (0.2794 cm).

```
1.257E-2/
      CR52
0
   1
      NI58
              5.479E-3/
0
   1
      MN55
              1.01E-3/
0
   2
      U235
              3.36E-5/
0
   2
      U238
              1.572E-2/
0
   2
      016
              4.724E-2/
0
   3
      NA23
              2.235E-2/
0
   4
              4.724E-2/
      016
0
   4
      FE56
              3.215E-2/
0
   4
      MONAT
             6.3E-5/
0
   5
      FE56
              5.706E-2/
0
   5
              1.639E-2/
      CR52
0
   5
      NI58
             8.118E-3/
0
   5
      MN55
              1.41E-4/
0
   6
      PU239
             9.8506E-3/
0
   6
      PU240
             1.308E-3/
0
   6
      PU241
            1.473E-4/
0
   6
      U235
              6.17E-5/
0
   6
      U238
              2.7584E-2/
0
      MONAT
             2.498E-3/
   6
1
   6
      PU239
             8.8672E-4
                         CC/
   6
              1.1944E-4 CC/
1
      PU240
   6
      PU241
                         CC/
1
             1.33E-5
1
   6
      U235
             7.14E-6
                         CC/
   2
      U235
             5.46E-6
                         CC/
1
```

```
6
      U238
               2.5203E-3
                           CC/
1
   2
                           CC/
      U238
               3.2601E-3
1
              2.357E-4
1
   6
      MONAT
                           CC/
               9.290E-3
   3
      NA23
                           CC/
1
1
   4
       016
               8.947E-3
                           CC/
   2
1
       016
               5.033E-3
                           CC/
   5
      FE56
                           CC/
1
               1.26E-3
               5.929E-3
   4
      FE56
1
                           CC/
1
   1
       FE56
               5.778E-3
                           CC/
1
   5
       CR52
               4.96E-4
                           CC/
1
   1
       CR52
               2.213E-3
                           CC/
               2.27E-4
1
   5
       NI58
                           CC/
   1
       NT58
               1.013E-3
                           CC/
1
               3.9E-5
1
   5
       MN55
                           CC/
   1
       MN55
                           CC/
1
               1.73E-4
2
   7
       U235
               8.56E-5/
2
   7
       U238
               3.96179E-2/
2
   7
       MONAT
               3.8E-6/
2
   7
       016
               2.4E-5/
2
   7
       FE56
               4.637E-3/
2
   7
       CR52
               1.295E-3/
2
   7
       NI58
               5.635E-4/
2
   7
               9.98E-5/
      MN55
CHI
STOP
```

This run is similar to problem 7 except that additional regions are defined for the infinite slab model of the core cell. These regions have IMIX=0 so that their cross-sections are not written onto the output file. However, the macroscopic cross-section for each region is calculated and used during the self-shielding iteration. To compute the Dancoff correction, the code sums up the optical path to the left from one region containing a particular material to the next region containing the same material, and then it does the same thing to the right. In either case, if the sum gets to the cell edge before the "black" region is found, the optical path is doubled to account for the reflective boundary condition. If the left optical path is zero, it is set equal to the right path; the complementary procedure is used if the right optical path vanishes. Therefore, both symmetric and asymmetric two-region equivalent cells are formed.

It is clear from the way the multiregion cell was constructed that the homogenized core cross sections cannot be computed by homogenizing regions 1 through 5 directly. In addition, the material loadings varied from cell to cell in the actual assembly; and other structure, instrumentation, and control regions also contributed to the net densities for the assembly. TRANSX handles this problem by defining the core mix using the constituent cross sections from regions 1-5 but using the homogenized densities from the homogeneous model. When a particular isotope

occurs in several different regions, the homogenized density is apportioned between them (e.g., 81.7% of the 304 stainless steel is in region 1, and 18.3% is in region

5 with different background cross sections). The CC command is used to request constituent cross sections because these densities are cell-averaged densities.

The model used in this example accounts for the heterogeneous self-shielding effect, but not for the advantage and disadvantage effects. They can be obtained by using a flux solution by regions to do a flux and volume weighting of each cross section in the assembly. This can be done using two TRANSX runs and an  $S_N$  code as shown below. These examples also illustrate how to use thermal upscatter cross sections.

### F. Self-Shielded Thermal Reactor Problems

Thermal neutrons are usually important when light materials (for example, water or graphite) are present. Such problems are characterized by the presence of upscatter. In addition, thermal assemblies are often strongly heterogeneous because of high absorption cross sections. Thermal upscatter cross sections are available on some of the MATXS libraries (see Section V), and the heterogeneity is usually treated by fine-group structures and/or heterogeneous self-shielding methods.

Sample Problem 9. Homogenized Thermal Critical Assembly

```
TEST 9 -- ORNL-1 BENCHMARK
       1 1 1 0
                   3
      93 20 40 1 1 7
GLOP
GLOP
     300. 1. 1 34.595/
     H1
        .066228 H20/
     016
         .033736 FREE/
     N14 1.869E-4 FREE/
     U234 5.28E-7 FREE/
     U235 4.8066E-5 FREE/
1
  1
     U236 1.38E-7 FREE/
  1
     U238 2.807E-6 FREE/
CHI
STOP
```

This benchmark is modeled as an homogeneous sphere of uranyl nitrate in water without a container.  $^{17}$  It is important to use a MATXS library like one of the 69-group libraries that has both upscatter cross sections and self-shielding factors. Note that 20 upscatter groups are allowed, for a total table length of 4+69+20 = 93 groups. Using 40 thermal groups gives a thermal cutoff of 2.60 eV; that is, there is no upscatter to groups above this energy. The self-shielding treatment accounts for the mixture effects and the possibility of escape from the sphere (the mean

**Table 3:** Moderator materials on the ENDF/B-VI thermal data files. The names in parentheses give the binding state for the principal scatterer. For example, C in graphite, or H in water. The MATXS names are based on this binding condition. Elastic scattering can be either coherent (coh) or incoherent (iel). In either case, the MATXS name is constructed by appending a dollar sign (\$). The last column gives the appropriate treatment to use for the secondary atom, if any (see text).

Material Name	MATXS Name	Elastic Treatment	Secondary Treatment
Be	BE	coh	
${ m BeO}$	BEO	$\operatorname{coh}$	none
C(graphite)	GRAPH	coh	
C(polyethylene)	POLY	iel	free C
$C_6H_6$	С6Н6		none
$D(D_2O)$	D2O		free O
$H(H_2O)$	H2O		free O
$\operatorname{Zr}(\operatorname{ZrH}_n)$	ZRH	iel	$\mathrm{H}(\mathrm{ZrH}_n)$
$H(ZrH_n)$	ZRH	iel	$\operatorname{Zr}(\operatorname{ZrH}_n)$

chord length is 34.595 cm). Free-gas thermal scattering is used for all materials except hydrogen, which is bound in water.

Most ENDF/B-VI thermal evaluations give the scattering from an atom as bound in a molecule or crystal lattice, and the effects of the different atoms in a molecule must be combined in TRANSX to obtain the net thermal scattering cross sections. As an example, water in the sample problem above is a combination of H bound in H<sub>2</sub>O and free-gas oxygen. However, some ENDF/B evaluations give the scattering for the entire molecule in the tabulation for the principal scatterer. In these cases, the thermal cross sections are renormalized to be used with the principal scatter. The TRANSX user must be careful not to include free-gas scattering for the secondary atoms. Table 3 lists the thermal evaluations available in ENDF/B-VI and indicates which treatment of secondary atoms was used. This table also indicates which evaluations require both inelastic and elastic parts. The elastic names (whether coherent or incoherent) are obtained by appending a dollar sign (\$) to the names given.

As examples, the TRANSX material specifications for graphite, beryllium oxide, methane, and ZrH might take the forms

```
1 1 CNAT 1. GRAPH GRAPH$/
2 2 BE9 1. BEO BEO$/
```

```
016
         1.
             NONE/
         6.
             C6H6/
3
   H1
   CNAT
         6.
             NONE/
   H1
             ZRH ZRH$/
         1.
   ZR
         1.
             ZRH
                   ZRH$/
```

For self-shielding problems like this one, it is necessary to define a mixture in order to calculate the  $\sigma_0$  values. However, the user often needs the "constituent" self-shielded microscopic cross sections for such applications as concentration searches or depletion calculations. These constituents can be requested by defining additional output mixes and by using mix specifications containing the key words "CC" (for cell constituent) or "RC" (for region consituent). Sample problem 9 would become

```
.
.
69 2 93 20 40 8 1 14 1 0
GLOP H1 016 N14 U234
U235 U236 U238
.
.
.
1 1 U238 2.807E-6 FREE/
2 1 H1 1. CC/
3 1 016 1. CC/
.
.
8 1 U238 1. CC/
STOP
```

The entry "CC" tells the code to use the microscopic cross section that was added into the mix by the normal mix specification for this material and region. (The "CC" and "RC" commands are equivalent for a homogeneous case like this one.) The transport code now has the choice of using the macroscopic cross section or remixing using the micros. If the densities in a concentration search were to vary enough to change the self-shielding, it might be necessary to repeat the TRANSX calculation for the new mix.

Sample Problem 10. TRX-1 by Regions

```
TEST 10 -- TRX-1 REGIONS

0 5 0 1 2 1 0 3 0 0

69 2 96 20 40 3 3 5 4 3

FUEL CLAD MOD

FUEL 300 .75892 3 1.15 1.15/
```

```
CLAD
     300 .280851 -3/
MOD 300 1.78489 -3/
    U235 6.253E-4 FREE/
     U238 4.7205E-2 FREE/
     AL27 5.1728E-2
                    FREE/
3
  3
    H1 6.676E-2 H20/
  3 016 3.338E-2 FREE/
CHI F238 F235 C238
  NFTOT
        1 U238
  NFTOT 1 U235
4 NG
     1 U238
STOP
```

The TRX-1 thermal benchmark<sup>23</sup> is a hexagonal lattice of aluminium-clad pins of enriched-uranium in water. The heterogeneity option IHET=3 is used to compute the Dancoff corrections for an infinite hexagonal lattice. A 69-group library is used because it contains thermal scattering matrices. Note that free gas scattering is called up for most of the materials, but the cross sections for hydrogen in water are used for H1. Using 40 thermal groups gives a cutoff at 2.60 eV. Upscatter is limited to 20 groups; any larger energy gains would be truncated so as to preserve the scattering cross-section. The table length is 20+69+3+4, so all downscatter groups will be kept.

The output  $P_1$  cross sections are written in group ordering on a file in GOXS format, which can be read directly by the ONEDANT  $S_N$  code if its name is changed to MACRXS. Another copy of this file must also be made with the name SNXEDT for use by the ONEDANT edit module. The ONEDANT input for this case follows:

```
1
TRX-1 INFINITE LATTICE CELL - 69 GROUPS - ENDF/B-VI
DIMENS= 2 69 8 3 3 3 4 40 T
XMESH= 0. .4915 .5042 .5753 .9482 XINTS= 17 3 3 17
ZONES= 1 0 2 3 T
LIB= MACRXS T
ASSIGN= MATLS T
SOLIN= 1 1 0 0 3 SOLOUT= 1 0 0 0 0 0 0 1 NORM= 1. T
RZMFLX= 1 T
```

Note that no mixing is done in ONEDANT because the MACRXS file already contains the appropriate macroscopic cross sections for the two regions. The two key statements are LIB=MACRXS and ASSIGN=MATLS. When the flux calculation is complete, ONEDANT writes a flux file that can be used as input to a second TRANSX run. The RZMFLX file is a nonstandard CCCC file for regular zone moments flux (see Section IV).

## Sample Problem 11. TRX-1 Infinite Lattice Cell

```
TEST 11 -- TRX-1 INF. LATTICE CELL
    0 1 2 1 0 3 69 3
0 5
2 2
     10 40 1 1 3 5 4
CELL
FUEL 300
         .75892 3 1.15 1.15/
         .28085 -3/
CLAD
     300
MOD
    300 1.78489 -3/
    U235 6.253E-4 FREE/
     U238 4.7205E-2 FREE/
     AL27 5.1728E-2 FREE/
  3
     H1 6.676E-2 H20/
    016 3.338E-2 FREE/
  3
CHI F238 F235 C238
  NFTOT
        1 U238
  NFTOT
        1 U235
        U238
4 NG
     1
45
   24/
STOP
```

The entire self-shielding calculation is repeated, but this time everything is homogenized into IMIX=1 using the given volumes and the computed region flux moments from the RZMFLX file. Note that the results are collapsed into two groups. The resulting breakpoint will be at 0.625 eV so that the response edits can be used to calculate the epithermal-to-thermal ratios usually quoted for thermal critical assemblies. These two-group cross sections could also be used to calculate the net leakage from the system using a two-dimensional RZ transport code, thereby determining whether the basic cross-section set gives a multiplication close to critical.

#### IV. INTERFACE FILES

TRANSX uses interface files for cross-section input, flux input, and cross-section output. Some of the output files are simple card-image files, but the interface files<sup>25</sup> follow the pattern of the CCCC interface files.

## A. The MATXS Generalized Cross-Section File

The standard CCCC files, ISOTXS, BRKOXS, GRUPXS, DLAYXS, and ISOGXS, have a number of shortcomings that have made them difficult to use outside of the fast-reactor community where they were developed. ISOTXS is limited to a particular set of reactions that is inadequate at the higher energy found in fusion problems; it does not allow for such important supplementary information as heating (KERMA) and damage energy cross sections, and it does not allow for the partial cross sections needed for sensitivity analysis. BRKOXS doesn't provide for self-shielded group-to-group scattering cross sections. ISOGXS has the same problems as ISOTXS. There is no format for delayed photons or decay heat. These files use different formats to represent data that are basically similar, so the overhead of coding required to use them is high.

The MATXS format was designed to generalize and simplify the existing files. The first design principle was that all information would be identified using lists of Hollerith names. As an example, if the list of reactions included in the file contains entries such as NF, NG, and N2N, it is trivial to add additional reactions such as KERMA or DPA. The second design principle was that the file would be designed to hold sets of vectors and rectangular matrices and that the same format would be used regardless of the contents of the vectors and matrices. As a consequence, once a code is able to handle  $n \leftarrow n$  matrices, it can also handle  $\gamma \leftarrow \gamma$  data; once a code can handle  $\gamma \leftarrow n$ , it can also handle  $n \leftarrow \gamma, \beta \leftarrow n$ , or even  $p \leftarrow d$ . It was originally decided to divide the file into "data types" identified by its input and output particles. As an example,  $\gamma \leftarrow n$  is a data type characterized by input particle equals neutron and output particle equals photon. The matrices contain cross sections for producing photons in photon group  $n_q$  due to reactions of neutrons in group  $n_n$ . The vectors, if any, would contain photon production cross sections versus neutron group. Then, each data type was divided into materials and submaterials. A material might be a particular isotope or mixture (e.g., U238 or SS304). Each submaterial could then represent a particular temperature and background cross section in a basic library, or perhaps a particular region for a reactor. Starting with NJOY 91.0. this organization was changed to have the material as the outermost loop. Each material was then divided into submaterials, where each submaterial could belong

Name	Definition
N	Neutron
G	Photon (gamma or x-ray)
P	Proton
D	Deuteron
Т	Triton
Н	$^3\mathrm{He}$
A	Alpha ( <sup>4</sup> He)

**Table 4:** Particle types defined for current MATXS libraries.

to a given data type and have a given temperature and background cross section. This organization makes it much easier to add, delete, or extract materials from MATXS files. The MATXS library format that resulted from following these general principles is described in Appendix B. The standard CCCC form is used.

As in all CCCC-type files, a MATXS library starts with a **file identification** record that gives the name of the file, a user identification string, and a version number. This is followed by the **file control record**; here NPART refers to the list of particles found in the file (e.g., N, G, B); each particle has its own distinctive group structure. NTYPE is the count of data type names, and NHOLL is the count of words in a general description of the contents of the file, processing methods, accuracy criteria, and so on. NMAT is the number of materials given in the library. MAXW is the maximum size of a record to be found in the file. It helps in establishing storage requirements. Finally, LENGTH gives the total number of records in the library.

The file data record gives the particle and data type names (see Tables 4 and 5), the names of the materials, and the number of groups for each particle. It also characterizes each data type by identifying its input and output particles. Finally, it gives the number of submaterials for each material and the LOCM vector. The LOCM vector makes it easy to skip directly to a desired material without reading all the intervening data.

Each material starts with a **material control record**, which gives the name of the material and information on the submaterials. Once again, it is possible to jump directly to a desired submaterial by using the LOCS vector.

The first record for each submaterial is the **vector control record**. The vector data are organized by reactions with Hollerith names (HVPS). To keep the

Name	Definition
NSCAT	Neutron scatting
GSCAT	Photon scattering
NG	Photon production
NTHERM	Thermal neutron scattering
PSCAT	Proton scattering
PN	Proton-to-neutron matrix
NP	Neutron-to-proton matrix
•••	etc.

**Table 5**: Data types defined for current MATXS libraries.

maximum record size reasonable, the vectors can be given in several blocks; each vector is taken to be nonzero only between the given limits (NFG, NLG). Thus, excess zeroes are omitted for threshold reactions or for reactions with no high-energy groups such as thermal scattering. Any reaction that can be named can be stored in MATXS.

The convention used for naming most reactions is clear from the example in Appendix H (e.g., NG, NA, or N2N). The symbols NWTO, NWT1, NTOTO, and NTOT1 refer to the flux- and current-weighted components of the library weight function and the neutron total cross section. Fission may be split into the partial reactions NF, NNF, and N2NF; in any case, NFTOT is the total fission reaction. Discrete-inelastic scattering in ENDF is denoted by the level plus 50; thus, MT51 is  $(n, n'_1)$ . On the MATXS library, this is given as NO1. If the level decays by particle emission, the particle identifiers are tacked on after the number (e.g., N62DAA). Emission of <sup>3</sup>He is denoted by H.

The neutron files also contain some special quantities. HEAT and DAME are the local heat production and damage energy production cross sections. NUBAR, XI, GAMMA are the continuous slowing-down parameters. INVEL is the group-averaged reciprocal velocity. Finally, NUD and CHID are for delayed fission as described in Sec. II-B.

In the thermal data type, reaction names identify the binding condition; FREE for free gas, H2O for light water, D2O for heavy water, POLY for polyethylene, BENZ for benzene, GRAPH for graphite, ZRHYD for zirconium, and BEO for beryllium oxide. The elastic part is distinguished from the inelastic part by a \$ sign on the end of the name.

In the photon interaction data type, the reactions are GWTO, GTOTO, GHEAT, and GDAME analogous to the neutron names, GCOH for coherent scattering, GINCH for incoherent scattering, GPAIR for pair production, and GABS for photoelectric absorption.

After the vector blocks comes the matrix control record. The representation used for cross-section data is similar to ISOTXS in that it packs the data as bands of source groups that scatter into each given sink (final) group.

The matrix names used in the current libraries are the same as for the corresponding vectors. All the partial scattering matrices are kept separate for maximum flexibility. If groups of these partial matrices were to be combined by an auxiliary program, new names would have to be defined such as TOTAL or INELAS.

Summary descriptions of several existing MATXS libraries will be found in Section V. These libraries were derived from ENDF/B-V and ENDF/B-VI; they use neutron group structures with 30 to 187 groups and photon structures with 12 or 24 groups.

# B. RTFLUX, RZFLUX, RMFLUX, and RZMFLX Files

Four different flux input files are allowed. RTFLUX is a CCCC standard interface file<sup>25</sup> for regular total flux, which is normally used to give the  $P_0$  flux by fine mesh interval. TRANSX uses it as if it contained region or coarse mesh fluxes; if only one region is defined, RTFLUX is a handy way to pass central flux into TRANSX from a CCCC standard code. RZFLUX is a similar CCCC file for regular zone averaged flux.

What TRANSX really needs are the  $P_0$ ,  $P_1$ ,... moments of the flux given by coarse mesh regions. However, as all  $S_N$  codes have  $\phi_0, \phi_1, ...$  available from the calculation of the source term, the moments can be made available for output in a moments flux file. The ONEDANT and TWODANT codes now have the capability to write the RMFLUX (regular moment flux) file by fine mesh or RZMFLX (regular zone averaged moment flux) by coarse mesh. The format of these non-standard CCCC files is the same and is given in Appendix E.

It should be noted that ordering of the flux moments becomes more complex for cylindrical or two-angle plane geometry when the associated Legendre functions appear in the formulas. A good discussion of the ordering used in the Los Alamos transport codes appears in the ONETRAN report.<sup>26</sup> TRANSX should be limited to  $P_1$  sets for these cases.

### C. CARD 6E12 Format

This is a simple material-ordered card format that can be read by almost all transport and diffusion codes. The output file starts with a block for the first Legendre order of the first material, then gives the second order, third order, and so on. The file then continues with the first order of the second material, etc., until all the data blocks have been written.

Each block starts with a simple header card that gives the material name, Legendre order, table length, and number of groups. The data are then given using a 6E12.5 format starting with position 1 of final group 1, position 2, position 3, ..., up to position NTABL of the first group. The data then continue with all the positions for the second group, etc., until the block is complete. Each block contains NTABLxNGROUP words, six per line, with a sequence number on each line. An example of this format is given with the Sample Problem 1 output in Appendix A.

### D. CLAW Format

This is also a material-ordered format very similar to IOUT=1. The NED+3 edit positions are written out in a separate response edit block with its own header card containing the name of the material and the word "EDITS." All the groups for position 1 are written first in 6E12.5 format. A reaction identifier and sequence number are added to each card in columns 73–80. The same process is followed for the rest of the edits. The first NED positions are then removed for each group of the scattering blocks, and the blocks are written out using 6E12.5 cards. Each card has its Legendre order and a sequence number in columns 73–80.

The edit tables are very easy to access with a text editor in this form, and the positions reserved for edits in the high-order tables have been removed for economy in transport code storage.

# E. FIDO Output

The transport tables for IOUT=1 and 2 are usually more than half zeroes. This waste of words on the input file can be reduced by using FIDO format in which a group of N zeroes is replaced by one entry that says "repeat zero N times". TRANSX uses fixed-field FIDO, which divides a 12-column field into a 3-column part and a 9-column field without a decimal or an E (e.g., 1234567-6 is 1.234567). A negative number or a number with a two-digit exponent field ends up with less precision. To obtain the repeat option, "nnR" is put into the 3-column field where nn is the number of times that the number in the field following R is to be repeated.

A table is terminated by an entry with T in column 3 of the 12-column field and every other column is blank.

The materials and scattering blocks are written in the same order as for IOUT=1, and a header card is provided for each block. The tables are much more compact but harder to read. Some FIDO processors are much more elaborate than this one, but TRANSX uses only the R and T options.

## F. ANISN Output

There has been a long tradition in which ORNL codes wrote the source term of Eq. (1) as shown, but Los Alamos codes kept a factor of  $(2\ell+1)$  explicit in the sum. The only difference between the FIDO and ANISN options is that ANISN tables include the  $(2\ell+1)$  appropriate for ORNL codes and FIDO tables leave it out, as required by the Los Alamos codes. Modern codes like ONEDANT often have options to read either type of table. An easy way to distinguish between them is to look at the scattering matrix for a high-energy group with almost delta-function forward scattering. Los Alamos tables will have  $P_0 \ge P_1 \ge P_2 \ge P_3$ .... The higher orders will tend to grow for ORNL tables.

# G. ISOTXS Output

As pointed out above, the ISOTXS format has some shortcomings as a general library format; however, it is well suited as an output format from TRANSX because many codes can use it as input. For the convenience of the TRANSX user, the ISOTXS format specification<sup>20</sup> is reproduced in Appendix F.

When selecting ISOTXS output, the edit names can be STRPL, SNGAM, SFIS, CHISO, SNALF, SNP, SN2N, SND, or SNT. The first and second must be present (TRD and NG, respectively), and SFIS must be present (if not zero) to allow  $\bar{\nu}$  to be calculated from  $\nu\sigma_f$ . The others are optional. As an example,

```
$ IOUT=6, NED=9, NEDS=9
...
CHISO STRPL SNGAM SFIS SN2N
SNALF SNP SND SNT/
1 CHI/
2 TRD/
3 NG/
4 NFTOT/
5 N2N/
6 NA/
7 NP/
```

```
8 ND/
9 NT/
```

The ordering of the names is not important. Note that the edit specifications for SND could load HEAT or DAME into the corresponding position rather than the (n,d) cross section. This kind of trick must be used with care because some  $S_N$  codes may calculate their particle-balance-absorption edit from SNGAM+SFIS+SNALF+SNF+SND+SNT-SN2N. A separate vector chi is computed for each isotope with fission, but no set chi vector or matrix is provided.

The output coding produces a total scattering matrix only. It uses the option in which a different "block" is used for each Legendre order. Subblocking is not used, so the scattering blocks each consist of a single record containing all source and sink groups for that order. No attempt is made to take full advantage of JBAND and IJJ to remove zeroes, but the matrices are triangularized and truncated using MAXUP and MAXDN for some savings in output file size.

The parameters AMASS through KBR in the isotope control record are set to zero.

# H. GOXS Output

As pointed out in Section II, group ordering is the natural organization of the cross sections in an  $S_N$  code. Using a group-ordered library file saves the time required to flip the data from material to group ordering, and it allows large group structures to be used.

The GOXS (pronounced go-ex-ess) file is described in Appendix G. It was designed as a CCCC-compatible binary file to provide an efficient internal cross-section representation for any  $S_N$  code. It is compatible with the MACRXS file used in ONEDANT and TWODANT.

Like MATXS, the GOXS format uses Hollerith names for materials and vector cross sections. Thus, the number and types of response-function edits that can be included are essentially unlimited. Also, the availability of names for materials and reactions enables the code designer to produce a very readable printed output.

As noted previously, most of the vector cross sections are not needed during the flux calculation but only at the end of the job when responses are computed. If the transport code being used has such a post-edit capability, the TRANSX user can run a separate edit job as in Sample Problem 4, and the GOXS output coding will prepare a short file with no scattering tables. This file is then compatible with the SNXEDT file used by the EDIT module of ONEDANT and TWODANT.

Scattering matrices on GOXS are packed using "bands" as in ISOTXS to minimize the number of zeroes on the file. It is also advantageous to minimize the number of zeroes in the memory region where cross sections are stored. The same JBAND and IJJ arrays can be used to pack the scattering data into memory, if desired. Thus, GOXS is just an image of the internal data representation of the transport code giving maximum efficiency in data transmission. ONEDANT and TWODANT use this feature of GOXS.

No card-oriented group-ordered format is provided because (1) no *de facto* standard such as FIDO exists, and (2) it makes more sense to convert the existing  $S_N$  codes to read GOXS.

### V. SOME MATXS LIBRARIES

MATXS libraries are produced from evaluated nuclear data in the ENDF/B format using the NJOY nuclear data processing system. <sup>12, 13, 14, 15</sup> As of version 2.0, the preferred libraries for TRANSX are based on ENDF/B-VI. However, several older libraries based on ENDF/B-V have been converted to the current version of the MATXS format also.

## A. MATXS10

This is a library with 30 neutron groups and 12 photon groups (30 x 12) that includes 117 materials from ENDF/B-VI. Photon production and photon interaction are included, but self-shielding isn't. The Legendre order for the scattering matrices is P<sub>4</sub>. The materials are given at a temperature of 300 K. A complete list of materials and reactions included can be obtained from an INDEX of the library (a partial listing of this index will be found in Appendix H).

MATXS10 was prepared with a fusion + fission + 1/E + thermal Maxwellian weight function. It is useful for many high-energy calculations, including criticals such as GODIVA. It works surprisingly well for many shielding problems for which resonance self-shielding is not too important. The library is compact, and TRANSX runs usually require only a few seconds on a fast computer.

#### B. MATXS5

This library is similar to MATXS10, except that it was generated from ENDF/B-V. It includes neutron data for 100 materials (including 13 Dosimetry isotopes), photon production for 65 materials, and photon interaction cross sections for 87 elements. Several special Los Alamos evaluations and a lumped fission product from the Westinghouse Hanford Engineering Development Laboratory (HEDL) are also included. See the INDEX for more details.

# C. MATXS11

This is an 80 x 24 library from ENDF/B-VI intended for fast-reactor analysis. However, the group structure and weight function used also make MATXS11 a reasonable choice for fusion studies and shielding calculations.

This library features extensive self-shielded cross sections for the temperatures 300, 400, 600, 800, 1200, 1600, 2000, 3000, and 4000 K. Background cross sections vary from infinity down to a lower limit that depends on the normal applications

of the materials. The Legendre order is  $P_5$  for both neutrons and photons. See the INDEX for a complete list.

The 24-group photon structure is much better than the 12-group structure for low photon energies and for energies around the annihilation peak at 0.5 MeV. It also does a better job of describing the high-energy "shoulder" of capture gammas in some systems. This can be important for heating calculations.

MATXS is more expensive to use than the 30 x 12 libraries, but it is capable of giving good results for a wider range of problems.

## D. MATXS6

This 80 x 24 library is similar to MATXS11, except that it was prepared from ENDF/B-V. There are 148 materials, including 72 with photon production.

#### E. MATXS12

This is a 69 x 24 library from ENDF/B-VI for light-water-reactor problems. It includes self-shielded cross sections for the important actinides. Thermal scattering data are given for all the materials, with bound scattering for the important moderators. The group structure has 42 thermal groups extending up to 4.00 eV.

### F. MATXS7

This is also a 69 x 24 library, but it is based on ENDF/B-V. There are 118 materials, including the most important fission products. Photon production is included for 42 materials.

# G. MATXS13

The MATXS13 library has 187 neutron groups and 24 photon groups for a limited number of materials useful for shielding problems. It includes neutron data, photon data, thermal data, and self-shielding data in one unified package.

The photon data are the same as in MATXS11, but the increased neutron accuracy leads to better calculations of capture, hence better photon spectra.

The thermal structure includes 55 groups below 4.45 eV, thereby providing better resolution around the 1-eV  $^{240}$ Pu resonance and more accuracy at energies below 0.0253 eV. The fine epithermal group structure tracks the slowing down of neutrons better than the coarse groups of MATXS12. As more materials are

added to this library, it will become an accurate general purpose tool for thermal problems.

Finally, for high-energy problems, the thermal groups can be collapsed out. The result will still have a finer group structure than MATXS10 or MATXS11, and it can be used to attack difficult problems that do not seem to converge with the simpler libraries.

# H. MATXS8

This library is similar to MATXS13, except that it was processed from ENDF/B-V. It is an 80-group library for fast-reactor and fusion-reactor problems.

### VI. PROGRAMMING DETAILS

#### A. Version Control

TRANSX is maintained using the UPD code,<sup>27</sup> which is similar in concept to the UPDATE code used on Cray and CDC systems. It keeps a history of changes to a computer code that is very useful as part of a Quality Assurance (QA) program. However, UPD is much simpler than UPDATE, thereby facilitating transport from system to system. This transportability is very important, because it ensures that one set of "updates" will produce the same code for compilation on all the target systems. With other systems used in the past, modifications sometimes behaved differently on different systems.

UPD reads two files. The file named SRC contains the base version of the source code for the program. This file can be broken up into separately named sections with "\*DECK name" cards. However, TRANSX uses only the single deck named "TRANSX." For simplicity, there is no counterpart to the binary "program library" used in the UPDATE system. The second file is called UPN, and it contains the commands to modify the base source file into a compiler input file for the current version.

The following example illustrates the features of the UPN file needed for maintaining the TRANSX code:

```
*CPL
*LST
*IDENT UP1
*/ 6 JAN 92 -- INCREASE SIZE OF MAIN CONTAINER ARRAY
*D TRANSX.182
      DIMENSION A(500000)
*D TRANSX.222
      NAMAX=500000
*IDENT VERS
*/ VERSION UPDATE FOR TRANSX
*D TRANSX.12
      VERS. 2.1 (6 JAN 92)
*D TRANSX.216
      DATA VERS/' VERS. 2.1 (6 JAN 92)'/
*IDENT UNICOS
*/ MACHINE-DEPENDENT CHANGES TO TRANSX
*/ FOR CRAY-XMP MACHINES USING UNICOS AT LOS ALAMOS
*/ ELAPSED TIME
*D TRANSX.3806
      CALL SECOND(TIME)
*/ DATE
*D TRANSX.3816
```

CALL DATE(HDATE)

\*/ WALL CLOCK TIME

\*D TRANSX.3826

CALL CLOCK(HTIME)

The first line of this example gives the command CPL, which causes a compiler input file named CPL to be written containing the updated program. The command LST causes a listing file named LST to be written. These listing files are a little easier to read than normal CPL files.

The first set of changes begins with the card \*IDENT UP1. The modified lines on the CPL or LST files will contain labels like UP1.2, UP1.3, etc. This particular "ident" changes two lines in order to increase the size of the main container array. The symbol "\*/" introduces a comment line. It is very important for QA purposes to include comments in each ident that describe the purpose of the change. It is also very important that each change be dated as shown.

The next ident updates the version label on the code listing and the version string that is written to every TRANSX listing file. The numbering convention used for TRANSX is suggested by this example. Including an ident called UP1 increments the TRANSX version to 2.1; UP2 would give 2.2; and so on. Note that the date from the last ident is transferred to ident VERS. This scheme will be used for all "official" changes to TRANSX. Users are free to make private changes using their own special ident names.

The third ident implements some machine-dependent changes. These changes will be discussed below.

The general format for the delete command is

## \*D line1,line2

If ",line2" is omitted, line2 is taken to be the same as line1. The actual values for the line references can refer to lines in the base code (e.g., TRANSX.234) or to changed lines (e.g., UP1.2). In general, any line label that appears on the current CPL or LST file can be used. The delete command causes the range of lines named to be removed, and any text following the command is inserted at that point in the file. The insert command has the form

### \*I line1

Any text following the command is inserted after the named line. There is also a "before" command:

that causes the following lines to be inserted before the named line. Other features of the UPD code and more details on its use will be found in the UPD report.

## B. Code Conversion

TRANSX is designed to be converted easily between long-word machines (CDC, CRAY) and short-word machines (IBM, VAX, Sun). All Hollerith variables begin with the letter "H" and can be defined to be double-precision with a statement like IMPLICIT REAL\*8 (H). Expressions for the lengths of arrays and pointers for the starting locations of arrays all use the parameter MULT, which is set equal to 1 if the machine word can contain 8 or more characters and 2 if not (an IBM word contains 4 characters). The input routine FREE contains a machine-dependent variable MACHWD for the number of characters per machine word (MACHWD=10 for CDC, 8 for CRAY, and 4 for IBM, VAX, or Sun).

Most of the changes required to go back and forth between short-word and longword machines are carried out automatically using the conditional capabilities of the UPD code. As an example,

```
*IF SW
IMPLICIT REAL*8 (H)
*ELSE
IMPLICIT INTEGER (H)
*ENDIF
```

The user only has to be sure to include the line "\*SET SW" in the UPN input file for the UPD run (put it before the first "ident").

After these changes have been made, there may still be some incompatible system calls connected with input/output, CP time, date, clock time, and fatal error handling. Fatal errors use subroutine ERROR, which can often be adapted to provide trace back information or to leave a "drop file" for later analysis by an on-line debugging code. The subroutine TIMER is used to obtain elapsed CP time in seconds. DATER is used to obtain a date string (which can be formatted in different ways as long as it contains only 8 characters; examples are "mm/dd/yy," "dd/mm/yy," or "ddmmmyy"). WCLOCK is used to obtain the wall clock time; that is, the time of day for the TRANSX run. UPD idents are provided for several common machines and operating systems. These decks can also be used as starting points in constructing the updates required for other systems.

The problems of input/output have been alleviated somewhat by FORTRAN-77, but some installers may still find incompatibilities. TRANSX uses the CCCC

standard<sup>25</sup> subroutines SEEK, REED, and RITE. Local optimized versions may be available at installations that use existing reactor-physics codes. RITE is used to write a binary record and is very simple. REED is used to read binary records, but the reads may be nonconsecutive. At Los Alamos, nonconsecutive reads are supported using forward and backward record skipping. On some systems (especially VAX), it may be more efficient to rewind and skip forward rather than to use the backspace command. The SEEK routine is used to connect external files by name to logical unit numbers. The FORTRAN-77 version used in the code should work for most systems.

The Los Alamos CTSS version of TRANSX uses the program card to assign the input, output, and tty units, and the FILEREP call to enable reassignment of units on the execute line (e.g., transx input=test1,output=out1). Some systems may require explicit OPEN statements for these units.

## C. Storage Allocation

TRANSX uses variable dimensioning and dynamic storage allocation for efficient use of available memory. If insufficient memory is available, paging and multiple passes through the library file are used. This allows very large transport sets to be produced, if necessary, at the expense of running time.

For material ordering, the code determines how many materials and Legendre tables can fit into the available storage. It then makes one pass through the library file, produces the cross sections for the first set of materials and orders, and writes them out on the output file. It then rewinds the data file and repeats the entire process for the second set of materials and orders. This process continues until all the desired materials have been produced. The minimum set is one Legendre order and one material; if this does not fit, group ordering can be used.

For group ordering, the code determines how many groups (NGMAX) can fit in memory at one time. It then makes one pass through the data file for each set of NGMAX groups, writing out the group cross sections after each pass.

This paging strategy allows TRANSX to be run on small machines if necessary, but if a large memory is available, the code will run much more efficiently. Storage is assigned to a single container array A with NAMAX words (NAMAX is 300000 in the Los Alamos CRAY version). The allocation can be changed easily by changing the two statements DIMENSION A(300000) and NAMAX=300000.

A similar scheme is used during the calculation of self-shielding  $\sigma_0$  values. Cross section data are read in for groups JGL0 to JGHI, the  $\sigma_0$  values are computed and

printed, and the code repeats the process for the next group range, JGLO to JGHI.

Part of the NAMAX words of storage is reserved for reading the records of the MATXS cross section file by the statement INMAX=6000. This should be sufficient for MATXS files prepared with the default value of MAXW (5000).

## D. Description of TRANSX

TRANSX begins by initializing MULT, the units for system input and output (5 and 6), the scratch unit used for self-shielding data (20), the storage sizes (see Section V-C), and the parameter N12, which determines the maximum line length for the printed output file.

1. User Input After printing a heading, TRANSX begins to read the user's input. Most values are stored in variables with the name given in the input instructions (e.g., IPRINT, NTABL) or in the container array A using a pointer named by prefixing L to the name from the input instructions [e.g., IMIX values are stored at A(LIMIX+1), A(LIMIX+2), etc.]. The exception is the heterogeneity data IHET, CHORD, etc., which are packed in the container array as they are read; the array with pointer LIHET locates the parameters for each region in the big array.

Several additional arrays are defined using the input data. LMCHK points to an array used to check whether any materials requested in the mix specifications were not found on the library (sometimes this means that the name was misspelled). LGTAB points to an array containing the coarse-group index for each fine group that is constructed from the slightly different representation used for input. IMIXR is the "real mix" index; it runs over the NMIXR mix specifications that are not flagged as constituent cross sections with the labels "CC" or "RC". A related array is ICONS, which points to the "real" mix command for each constituent mix command. The number and names of the unique materials found in the mix specifications are also determined (see NUNIQ and the array HUNIQ starting at LHUNIQ+1). The array JMIX contains pointers to the unique material for each mix specification (or zero if the material is a constituent material), and the array KMIX contains a counter that distinguishes between the subsequent occurrences of a unique material in the mix specifications. Finally, MAXU is the largest number of times any unique material occurs. It is used later for dimensioning the FGAM and FFIS arrays.

If a spatial collapse is indicated by the input mix commands, the flag ISPC is set. In addition, TRANSX computes the cell volumes CVOL from the region volumes RVOL given by the user. The ratios of the region volumes to the cell

volumes are used to correct the input densities for constituent cross sections to the proper cell "CC" or region "RC" basis.

Several other flags are associated with the edit input. KPOS is set equal to the position to be occupied by the fission  $\chi$  data. Similarly, NPOS is the position to be occupied by the transport-for-diffusion cross section TRD. LOCG is the first position of a range of positions reserved for gamma source groups. See the special edit input parameter GAM. The flags LSNGAM, LLSFIS, etc., which are stored in common ISOT, are used for CCCC ISOTXS output. They mark the positions used for the edits that will end up as ISOTXS principal cross sections.

TRANSX stores some variables as integers, some as real, and some as Hollerith strings. This can be done freely because the variables A, IA, and HA are all equivalent. However, some care must be taken with Hollerith variables for shortword machines because the first word of each double-precision or 8-byte word must be at an odd memory location. The equivalent TRANSX pointer must be even. Therefore, TRANSX uses logic like this:

```
LMIXN=NEXT

IF (2*(LMIXN/2).NE.LMIXN) LMIXN=LMIXN+1
LOCH=LMIXN/MULT
```

The pointer is guaranteed to be even, and A(LMIXN+1) points to the first half of the Hollerith variable denoted by HA(LOCH+1).

When the reading of the user's input is complete, the flux interface, if any, and the MATXS cross-section library are initialized by reading the first few records from each file. The group structures are checked against the input value for the number of coarse groups (NGROUP) and the number of fine groups (NFINE). With collapse, NFINE can be a number greater than or equal to NGROUP. The number of fine and coarse neutron groups is also extracted (NGNF, NGN). The group bounds and average velocities are saved (see LGRP and LVEL). MATXS libraries can have a special velocity vector that is retrieved later, but in case it does not show up, an estimate is made here using the given group bounds. If the elastic scattering correction option has been requested, the lethargy widths of the groups are computed and saved at pointer LETH, and space is reserved for the correction coefficients to be defined later (IESC, LGAMMA).

This version of TRANSX is capable of constructing extended coupled sets with three or more particles in addition to the normal neutron-photon coupled sets. The number of coupled particles NCPL is determined from the number of digits in the input parameter ISET. The NSHIFT array is constructed to contain the number of groups that must be shifted in the coupled set to find the data for the nth particle.

The IRF array is used later to flag when the weighting flux for each particular particle has been read in.

At this point, memory is allocated for the flux arrays. The Legendre components of the fine flux are stored as if they were in an array FFLUX(fine group, region, order). For no collapse, this array starts at LFLUX+1. If collapse is requested, a coarse-flux array of the form CFLUX (coarse group, mix, order) starts at LFLUX+1, and the fine-flux array starts at the location

### LFLUX+NGROUP\*NMIX\*(NLMAX+1).

The use of NLMAX+1 orders provides for the flux moments needed for inflow transport corrections.

If an input flux file has been defined, it is read following the comment "READ FLUX FROM INTERFACE FILE." If there are fewer than NREG regions on the input file, the last region is used to fill out the table. If there are not NL+1 orders on the file, the last order is used to fill out the table.

If self-shielding has been requested, the appropriate background cross sections and self-shielding factors are computed by calling subroutine SIGZER. This routine uses temporary storage defined with respect to the pointer LC. It writes its results on the scratch tape NSS=NSCR.

Next, storage is allocated for the scratch arrays. LCNORM points to the total fission neutron production used to normalize chi; that is, the denominator of Eq. (19). LPNU points to the array of prompt fission  $\bar{\nu}$  values. LDNU and LDCHI point to the delayed-fission data. LSFIS is a pointer for the microscopic infinitely dilute fission cross section of the current material. LSGAM is used for the microscopic infinitely dilute capture cross section. LFFIS and LFGAM are used to store the self-shielded cross sections for fission and capture. LABSC is a pointer to the array used to accumulate the particle-balance absorption by the direct method. And finally, LTERPT locates the array of interpolation factors used for temperature interpolation.

Next, the storage above LC is allocated for the cross-section table using different strategies for material and group ordering, as described in the preceding section. The maximum numbers of materials, orders, and groups that can fit into memory at one time are NMMAX, NLMAX, and NGMAX. The parameters IMLO, IMHI, ILLO, ILHI, JGLO, and JGHI are used throughout the code to decide which materials, orders, and groups get loaded into the accumulating cross-section array.

2. Main Processing Loop The code is now ready to begin a pass through the MATXS library accumulating the appropriate cross sections into the transport table. This is done by calling subroutine RMATXS. When the subroutine returns control to the TRANSX level, the accumulated cross sections for the current range of materials or groups are ready to be printed out or written to the desired output file.

All the material-ordered output options are given first inside a loop over output mix and order (IMLO to IMHI, ILLO to ILHI). The transport table in memory is stored starting at LC as if it were an array C(position, order, material, group). The "order" and "material" indices are often collapsed into the single variable JM, which takes on NJM=NLMAX\*NMMAX values. The logic required to extract data from the table is clear from the coding for printed output. The CARD, CLAW, FIDO, and ANISN output options use simple subroutines to generate the appropriate output. The design of the WISOT routine is described in Section IV-G. Note that TRANSX reacts to the specific edit names defined for ISOTXS (e.g., SNGAM, SFIS, SN2N, etc.) only. The pointers LLSFIS, LLSN2N, etc., tell where the corresponding cross sections are located in TRANSX memory. The scattering blocks are written using the same fixed size for all materials; no attempt is made to squeeze out additional zeroes. On the printed listing, the numbers are arranged as N12 columns. A programmer can easily change N12 to make the output look good on either a terminal or a line printer.

The group-ordered output options are produced next inside a loop over the range of groups in memory (JGLO to JGHI). Only printed and GOXS outputs are provided for group ordering, but other output options could be added at this point. The tables in memory have the form C(position, order, material, group) starting at LC. The logic needed to write the tables is fairly clear from the coding for printed output. The GOXS output routine WGOXS writes out all the response edits specified in the TRANSX input, but they are reordered so that the first four vectors are always  $\sigma_{\text{tot}}$ ,  $\sigma_a$ ,  $\bar{\nu}\sigma_f$ , and  $\chi$ . The transport cross section for diffusion TRD is written next if available. The scattering matrix is packed to minimize the number of zeroes written to the output file.

After completing the output for this range of materials, orders, and groups, TRANSX loops back to process the next set until all the requested tables have been produced. Final messages are printed (including the list of materials not found from LMCHK), files are closed, and the job terminates.

3. Reading the MATXS file When the RMATXS routine is entered, the accumulation arrays are zeroed, and the material loop is begun. The code checks whether each material on the MATXS library is needed; if not, it skips it entirely. The LOCM array and the random access capabilities of REED make this fairly efficient.

The MATXS material control record is read in to memory at pointer L2, and a new pointer L3 is defined. Note that the material control data stays in memory while this material is being processed. A loop over all the submaterials for this material is executed; that is, a loop over data type, temperature, and background  $\sigma_0$ . The first submaterial in each data type is called the "base material." By scanning up from each base material, the list of NTEMP temperatures TTEMP for this data type is obtained. On subsequent steps of the loop, the current type, temperature, and background cross section are extracted (ITYPE, TMAT, SMAT). All background cross sections except infinity (1.E10) are skipped in RMATXS because the self-shielding calculation has already been performed in SIGZER.

With the data type identified, the values that depend on data type are assigned. These values include the identity of the input particle and the number of input groups (JINP, NING), the identity of the the output particle and the number of output groups (JOUTP, NOUTG), and the offsets for shifting the data block in a coupled set (JC1, JC2).

With the temperature identified, the appropriate interpolation weight for this submaterial is computed. This version of TRANSX limits itself to linear interpolation. Because each material may occur in several different mixtures or regions, the interpolation weights are stored in an array TERPT versus mix specification index IMX. If this particular submaterial does not contribute to any mix or region, the parameter ITERPT has the value zero, and the entire submaterial can be skipped. Otherwise, the submaterial is processed by starting the code segment with the comment "PROCESS THIS SUBMATERIAL."

The vector reactions are processed first. The MATXS vector control record is read into memory at pointer L3, and a new pointer L4 is defined for the blocks of vector cross-section data. The general procedure is to loop over the complete set of reactions needed for the transport tables and edits. For each group, the selected cross sections are multiplied by TERPT and/or density and added into the appropriate storage location. If necessary, self-shielded cross sections from the NSS scratch file are substituted for the cross sections from the MATXS vector block. The additional factor RVF is used to correct constituent cross sections for the definition of the density used on input; they can be either cell densities or region

densities. See the block of coding after "GET GROUP CROSS SECTION." The model weight functions in the cross-section block are treated specially. The data for each particle are read into the WTM array using the offset JC1, and the WTREAD flag is set.

If an elastic scattering correction has been requested (INITF<O), the expansion coefficients representing the smoothed fine-group flux are computed (X1, X2, X3) and used to compute the value and slope of the the smoothed flux at the bottom of each group. The coefficients used later for the removal corrections are stored in the array ESCC. If self-shielded cross sections were prepared in SIGZER, an appropriate self-shielded model flux has already been prepared. If there is no flux input file, the FFLUX and CFLUX values are computed using the model weight functions.

Note that only the base submaterial is processed for self-shielded reactions in the non-thermal range because the self-shielded cross section already includes the effects of temperature. All submaterials for these reactions are processed in the thermal range. All submaterials for non-shielded materials are also processed. This allows the temperature effects to be incorporated by using the TERPT factors.

The block of coding that loads the  $\sigma_a$ ,  $\sigma_{tot}$ , and  $\sigma_{g \leftarrow g}$  positions is especially complex because of the transport correction options defined by Eqs. (7) through (13). The P<sub>0</sub> total is put into the  $\sigma_a$  position, and the correction defined by Eq. (21) is subtracted later while the scattering matrices are being processed. The contributions of the P<sub>0</sub> and P<sub>1</sub> total cross sections to the total and in-group positions are made here also, and the matrix contributions needed for the transport correction, if any, are added later.

The block of coding after the comment "FISSION CROSS SECTION" only comes into play for data that have not been self-shielded (normally the thermal data type). The variable FFIS thus includes the effect of temperature on  $\bar{\nu}\sigma_f$ .

The transport cross section for diffusion (TRD) is calculated next. The  $P_1$  total is added in here (or  $P_0$  if  $P_1$  is not available), and the total  $P_1$  scattering cross section is computed and subtracted later during matrix processing.

The thermal correction to the total cross section was described in Section II-J. Note that both the absorption and total positions are involved; if the reaction is elastic, the cross section is subtracted, and if the reaction is the coherent or incoherent one specified in the mix specifications, the cross section is added.

The final block of coding in the material loop adds in any contributions to the edit positions using the multiply-and-accumulate algorithm, which allows any linear combination to be calculated. After the material loop is complete, the scratch cross sections are saved. These are quantities characteristic of this particular submaterial that will be needed later in the vector loop for processing the scattering matrices, or for calculating steady-state fission. SFIS and SGAM contain the infinitely dilute fission and capture cross sections used in computing  $\bar{\nu}$  and the shielding factors for photon production. The scratch data DNU and DCHI are the delayed-neutron yield and spectrum, respectively. Finally, GAMMA is  $\gamma_g$  used in the elastic scattering correction defined by Eq. (38).

The reaction loop is continued until all the required vector reactions for this submaterial have been processed. Then the loop over the matrix reactions is started. Each matrix block (reaction) can be divided up into a number of subblocks. A subblock may be part of the main matrix, in which case it contains data for a range of final groups JL to JU that contains fewer than MAXW words. Or it may be a constant spectrum or production cross-section subblock. The coding after the comment "SCATTERING SUB BLOCKS" handles this loop over subblocks.

If the current submaterial is needed for one of the accumulating mixes, the code sets up a loop over final energy group (sink group), initial energy group (source group), and Legendre order. The group-to-group cross sections XSNOW for each order may contain a matrix part and/or a part computed from the constant spectrum and production vectors. If the reaction is elastic scattering, it may be replaced by a self-shielded cross section. Next, the thermal correction is made, if desired (the elastic scattering at low energies is replaced by the appropriate incoherent and coherent thermal scattering). The resulting group-to-group cross section is multiplied by the appropriate factor from TERPT to affect temperature interpolation, and, optionally, an elastic removal correction factor is applied.

Following the comment "GET TRANSFER CROSS SECTION," this final microscopic cross section XSNOW is converted to a macroscopic cross section (note the correction for cell or region densities implicit in the factor RVF) and multiplied by the flux ratios needed for collapse and homogenization. In addition, the neutron-photon matrices for capture and fission are self-shielded using the data in the FGAM and FFIS arrays.

Separate blocks of coding are provided to accumulate the transport matrix with truncation of the table, if necessary, to compute a photon source in the edit positions (GAM option), to finish the calculation of the particle-balance absorption  $\sigma_a$ , and to complete the transport cross section for diffusion. In the block labeled "FISSION VECTORS," the fission matrix is multiplied by the flux and summed

over source groups to get the prompt part of the numerator in Eq. (19). The same term is added to the array in CNORM to be used to normalize  $\chi$  later.

The last step in the reaction loop adds the prompt component of fission into the microscopic  $\bar{\nu}\sigma_f$  in PNU. When the reaction loop finishes, the data in PNU are promptly converted to  $\bar{\nu}$  by dividing by  $\sigma_f$ , which was saved at LSFIS during the processing of the vector cross sections.

After the end of the submaterial loop, all of the effects of self-shielding and temperature have been included in the cross sections. The contributions from this material to the prompt or steady-state values of  $\bar{\nu}\sigma_f$  are then added into the transport table. Any delayed contributions to CNORM, the denominator of the expression for  $\chi$ , are also added in here.

This process is continued until all materials have been processed. The fission  $\chi$  is then normalized using the data in CNORM. In addition, the particle-balance absorption in the transport table is compared with the directly-computed value in ABSC. If the value in ABSC is small with respect to the transport cross section but still will have a large effect on  $\sigma_a$ , it is used to replace the previous value of  $\sigma_a$ . The tables are now complete for the ranges of mixes, orders, and groups currently allowed in memory. RMATXS returns to TRANSX, so they can be printed and/or written onto the requested output interface file.

4. Self-Shielded Cross Sections The effects of self-shielding are computed in subroutine SIGZER, and the resulting self-shielded cross sections are written out onto the scratch file NSS. In order to allow for possible storage limitations, the calculation is done by "pages" of MAXGRP groups (see JGLO and JGHI). The input MATXS file is read once for each page of groups.

The file data is already in place at pointer L1, and each pass starts by looping over all the "real" materials needed from the MATXS library. The procedure is similar to the one used in subroutine RMATXS, except that only the total, elastic, capture, fission, and elastic downscatter cross sections are extracted. They are all stored in the array SIGS(ISIGZ,IX,IMX,IG), where the indices refer to the background  $\sigma_0$ , the reaction type, the mix specification, and the group index, respectively. Each cross section is interpolated to the temperature appropriate to IMX before being stored in SIGS. The code allows for up to 20 elastic scattering elements. For a  $P_4$  set, this corresponds to the in-group element and 4 downscatter terms.

Once all the cross sections for this range of groups have been read in, the  $\sigma_0$  values can be computed by iteration. The code begins a loop over all the "real" materials in the mix specifications. The current material IMX lies in region IRG, which determines the heterogeneity parameters to be used. The  $\sigma_0$  values for each group is computed in two parts. First, the mixture part is computed using Eq. (25), where the sum runs over all the other materials in IRG. The code then begins to calculate the escape part of  $\sigma_0$ .

For IHET=1, the simple result of Eq. (26) is used with an effective mean chord specified by the user.

For lattices of cylinders (IHET=2 through 4), a macroscopic cross section homogenized over the two regions outside the fuel is required. Because the fuel is in the first region, the loop sums the macroscopic cross section times volume for the next two regions, obtaining the desired average in SMOD. The rest of the calculation of the escape cross section is straightforward.

For the slab options (IHET=5 through 8), the sweep through the cell starts from IRG and moves to the right, summing the product of the macroscopic total cross section for each region times the thickness of the region. The sweep continues until a region containing the current material or the edge of the cell is reached. If the edge of the cell is reached, the sweep either jumps to the other end of the cell and continues to the right (periodic cells) or reverses direction and sweeps back to the left (reflective cells). When a region containing the current materials is reached, the code repeats the entire process sweeping to the left. The final results are XXR and XXL, which can be used for  $\lambda_R$  and  $\lambda_L$  in Eqs. (33) or (34). Note that regions at periodic boundaries have their full thickness, but only half the thickness is given for regions lying on reflection planes. The calculation of the escape cross section can now be completed using Eq. (35).

Finally, the escape part is added into  $\sigma_0$ , the new  $\sigma_0$  is checked against the previous value, and the loop over materials and groups is continued. If convergence to within EPSZ has been achieved for all groups and materials, ISOK will be one, and the loops will terminate.

The final steps after convergence are to print out the table of computed  $\sigma_0$  values by material and group for this range of groups, to write out the results to the scratch file, and to continue the loop over pages of groups.

#### E. Error Messages

The error messages written by TRANSX are listed below along with an analysis of the problem and recommended corrections.

### FULL TABLE REQUIRED FOR COUPLED SETS

It doesn't make sense to truncate a coupled set by giving a table length less than **3+NED+NGROUP** because this would remove parts of the n-gamma block. Increase the table length requested.

#### REGION INPUT ERROR

The region temperature has an unreasonable value. Check your input. This kind of thing can result from a missing "/" on a previous card.

#### MIX INPUT ERROR

Either IMIX or IREG has an unreasonable value. Check your input. Once again, there may be a missing terminator on a previous card.

#### NO CONSTITUENT CROSS SECTION MATCH

The code is unable to find a constituent cross section with the given material name in the given region. Check your input.

#### INCONSISTENT COLLAPSE

The number of fine groups found by adding up the NGROUP values given in the collapse specification (input card 10) must be equal to the number of fine groups entered in ICOLL on input card 2.

#### INCONSISTENT FLUX FILE

This message usually means that the group structure on the flux file does not agree with the structure implied by the TRANSX input file. It may also mean that this is a three-dimensional flux file.

#### INCONSISTENT GROUP STRUCTURE

The number of groups found on the input library for the various particles are not consistent with the input quantities NGROUP and NFINE. Sometimes this means that the wrong MATXS library was mounted. Otherwise, check the values of the parameters, especially for complex coupled sets.

#### STORAGE EXCEEDED FOR LSS

There is not enough storage available for the self-shielding calculation. Either reduce the number of mix specifications and/or the number of groups, or increase the size of the main container array. The instructions on how to do this are given at the beginning of this section.

#### INSUFFICIENT STORAGE FOR MATERIAL ORDERED FORM

This message means that not even one Legendre order of one material can fit in the available storage. Either change to group ordering (which is more appropriate for very large group structures), or increase the size of the main container array. See above.

### INSUFFICIENT STORAGE FOR GROUP ORDERED FORM

This message is unlikely considering the small amount of memory required to process a single group. It means that too much storage was consumed in flux arrays and scratch arrays. The only recourse is to increase the size of the main container array. See above.

#### ILLEGAL FORM

The IFORM variable can only take on the values 1 and 2. Any other value is illegal.

#### TEMPERATURE OR SIGMA ZERO MISMATCHED

This message comes from SIGZER. It results from trying to match the T and  $\sigma_0$  values for one submaterial with the list of possible T and  $\sigma_0$  values for all the submaterials in the material. It should not occur.

### SEEK--BAD OPTION hname nop

This version of SEEK does not handle "nop" values of 4 and 5, nop values outside the normal range 0–7, or the "change" option. This error should not occur for TRANSX.

#### SEEK--FILE DOES NOT EXIST hname

For the "read seek" option, the file "hname" must already exist in your local file space.

#### SEEK--NO UNITS AVAILABLE hname

Seek assigns unit numbers between 10 and 19. This error means that more than 10 units are open. It should not occur for TRANSX.

## VII. Using BBC

BBC is a utility code for maintaining MATXS libraries. It can be used to convert them back and forth between binary and BCD (*i.e.*, formatted) modes, to selectively list the contents of a library, or to construct an index to the materials and reactions on a library. It can also be used to modify a MATXS library in several ways. It can select a subset of the materials from a library in order to make a new smaller library (smaller libraries run faster with TRANSX). The select option could also be used to list the cross sections for a particular material, if desired. BBC can insert new materials into a library or delete old materials. The select and insert capabilities can be used together to combine the information from two MATXS libraries. Finally, BBC can edit the MATXS version number, user identification, and file identification information.

### A. BBX Input Instructions

The input instructions follow. They were copied from the comment cards near the start of the BBC source file.

```
CARD 1
     IINPF
               INPUT FILE TYPE
                  1 BINARY (NAME = MATXS)
                 -1 CODED (NAME = TEXT)
     IOUTF
               OUTPUT FILE TYPE
                  O NONE
                  1 BINARY (NAME = MATXS OR MODOUT)
                 -1 CODED (NAME = TEXT OR MODOUT)
     IMODF
               MODIFY FLAG
                    NO MODIFICATIONS (DEFAULT)
                  1 MODIFICATIONS GIVEN
     LIST
               LIST OPTION
                  O NOT LISTED
                  1 LISTED (DEFAULT)
               INDEXING OPTION
     INDX
                    NOT INDEXED
                     INDEXED (DEFAULT)
                  1
CARD 2
         (LIST.NE.O ONLY)
     IRD
               RECORD TYPE PRINT FLAGS.
                  1 FILE IDENTIFICATION
                    FILE CONTROL
                     SET HOLLERITH IDENTIFICATION
                  4 FILE DATA
                  5 GROUP STRUCTURE
                    MATERIAL CONTROL
                  7 VECTOR CONTROL
```

- 8 VECTOR BLOCK
- 9 SCATTERING MATRIX CONTROL
- 10 SCATTERING SUB-BLOCK
  ONE VALUE FOR EACH RECORD TYPE

O NOT PRINTED, 1 PRINTED.

CARD 3 (IMODF.NE.O ONLY)

HOPER MODIFY OPTION

- S SELECT MATERIALS FROM MATXS INPUT FILE
- I INSERT MATERIALS FROM MODINP FILE

HMAT1 FIRST MATERIAL IN RANGE

HMAT2 LAST MATERIAL (DEFAULT=HMAT1)

REPEAT CARD 3 UNTIL A BLANK LINE IS READ

CARD 4 (IMODF.NE.O ONLY)

NEWVER NEW FILE VERSION NUMBER

HUSER NEW USER ID STRING (UP TO 16 CHARS)

CARD 5 (IMODF.NE.O ONLY)

HLINE LINE OF NEW HOLLERITH ID DATA (72 CHAR MAX)

REPEAT LINE 5 FOR EACH LINE OF THE NEW HOLLERITH DATA BLOCK. TERMINATE WITH AN EMPTY LINE. IF NO LINES ARE READ, THE ORIGINAL BLOCK IS UNCHANGED.

Because binary libraries cannot normally be moved between different computer systems, the MATXS file specification includes formatted version of each different record type (See Appendix B. Therefore, BBC includes the capability to convert files back and forth between BCD and binary modes. The simplest input to go from binary to BCD would be

1 -1 0 0 0

and to go from BCD to binary,

-1 1 0 0 0

The binary unit (input or output) is always called "MATXS", and the BCD unit (input or output) is always called "TEXT." It is often useful to make a partial listing and an index at the same time as a binary to BCD conversion. This can be done using

1 -1 0 1 1 1 1 1 1 1 1/

The partial listing on the file named OUTPUT will contain only the first five records of the MATXS library, namely, file identification through group structures. The index listing will appear on the file named INDEX.

The cost of running TRANSX can be reduced substantially by preparing a condensed version of a MATXS library that contains only the materials of interest. For example, a special library to run the TRX benchmark calculations could be prepared using the following input:

```
1 1 1 0 0
S H1/
S 016/
S AL27
S U235/
S U238/
/
112 *T2LANL BBC*/
*SHORTENED VERSION OF MATXS12*/
*FOR TRX BENCHMARK CALCULATIONS*/
/
```

The original library should be MATXS12 with its name switched to MATXS. The version number is changed to 112, so it would be convenient to change the name of the MODOUT file to MATXS112.

When it becomes necessary to update an isotope on an existing MATXS library or to insert a new isotope into the library, it is inconvenient and expensive to repeat the entire process of preparing the library using the MATXSR module of NJOY. An alternative approach is to prepare a small MATXS library containing only the new material, and then to add it to the library. Assuming that the MATXS10 library has been copied to the file MATXS, and that a new version of the <sup>11</sup>B data is on unit MODINP, you run BBC using the following input:

```
1 1 0 0 1
S H1 B10
I B11/
S CNAT ES253 /
10 *T2LANL BBC*/
```

Note that <sup>11</sup>B is replaced and that the original version number and Hollerith descriptive text are used for the new library. The output file MODOUT should then be switched to MATXS10 and used to replace the previous version.

#### B. BBC Error Messages

The error messages than can result when running BBC are listed below along with recommended actions.

#### INPUT MUST BE BINARY FOR MODIFICATIONS

Because modifications can be specified in any order, it is necessary to use binary files for both MATXS and MODINP. The random-access capabilities of REED can then be used to jump to the desired materials. Existing BCD files can be converted to binary using separate BBC runs before the modification run is made.

#### TOO MANY MATERIALS, CHANGE NUCS

Several arrays that depend on the number of materials are dimensioned by NUCS. If more materials are needed, this number can be increased by changing NUCS=200 in the parameter statement at the start of BBC.

### TOO MANY VECTORS, CHANGE NVEC

Several arrays that depend on the number of reaction names are dimensioned by NVEC. If more names are needed, this number can be increased by changing NVEC=150 in the parameter statement at the start of BBC.

#### SEEK--BAD OPTION hname nop

This version of SEEK does not handle "nop" values of 4 and 5, nop values outside the normal range 0–7, or the "change" option. This error should not occur for BBC.

#### SEEK--FILE DOES NOT EXIST hname

For the "read seek" option, the file "hname" must already exist in your local file space.

#### SEEK--NO UNITS AVAILABLE hname

Seek assigns unit numbers between 10 and 19. This error means that more than 10 units are open. It should not occur for BBC.

### VIII. ACKNOWLEDGMENTS

The author would like to thank the TRANSX users who have helped to find and fix problems in the code over the years since its introduction. More recently Denise George has made significant contributions to TRANSX and did much of the rewrite of BBC.

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## Appendix A. SAMPLE OUTPUT LISTINGS

O NUMBER OF THERMAL GROUPS
3 MIXES OR MATERIALS

6 MIXTURE SPECIFICATIONS

1 EXTRA EDIT POSITIONS

1 EDIT SPECIFICATIONS

1 REGIONS

This appendix shows portions of the output listing from Sample Problem 1, the "CARDS" output from Sample Problem 1, the output listing from Sample Problem 2, and the "FIDO" output from Sample Problem 3. The parts that were removed are indicated with ellipses.

## Sample Problem 1

```
VERS. 2.0 (2 JAN 92)
TRANSX
TRANSPORT CROSS SECTIONS
                                              RAN ON 01/22/92
                                                 AT 14:52:05
FROM MATXS LIBRARIES
                   _____
TITLE
TEST 1 -- MATERIAL ORDERED TABLES
OPTIONS
_____
IPRINT O (O=LONG/1=SHORT)
1 (0=NONE/1=CARD/2=CLAW/3=FIDO/4=ANISN/5=GOXS/6=ISOTXS)
ITRC 3 (O=NO TRANSPORT CORR/1=CONS.P/2=DIAG/3=B-H-S/4=INFLOW)
ICOLL
       O (O=NO COLLAPSE/NFINE=COLLAPSE)
INITF
         O (O=LIBRARY FLUX/1=PO CARDS/2=RTFLUX/3=RZMFLX/NEG FOR ESC)
PARAMETERS
NGROUP
        30 GROUPS
NL
     2 TABLES
NTABL
        34 POSITIONS IN TABLE
       O UP SCATTER GROUPS
NUP
```

#### MIX NAMES

NTHG NMIX NREG

NMIXS NED

NEDS

- \_\_\_\_\_
- 1 CARBON
- 2 TUNGST
- 3 U-235

REGION		TEMP(K)	SIZE	HETEROGENII	ETY		
1		3.000E+02	1.000E+00	0			
SPEC M	IX RE	G NUCLIDE	DENSITY	THERMAL	MATRIX	MOD	
1	 1 1	CNAT	1.000E+00				
2	2 1	W182	2.630E-01				
3	2 1	W183	1.430E-01				
4	2 1	W184	3.070E-01				
			2.860E-01				
6	3 1	U235	1.000E+00				
EDIT N	AMES						
1 H	EAT						
EDIT S	PECIFI	CATIONS					
1 H	 EAT	 1.602E-1	9				
INPUT 1	MATYC I	CTT C					
WORDS .	AVAILA OF OU	BLE FOR TA	SECTION TAEBLE = 6120 RES PER PASS ERS PER PASS	:= 3			
							0.1S
FINE F	LUX FO	R REGION	1 SUM 3.4	:360E+07			
3.72	3E+03	7.392E+04	1.905E+04	1.410E+04	2.312E+04	4.396E+04	
5.40	8E+05	1.176E+06	1.031E+06	7.341E+05	5.809E+05	1.156E+06	
	5E+06	1.154E+06		1.154E+06	1.155E+06	1.155E+06	
** CAR	BON PO	**					
POSITI	ON	GROUP 1	GROUP 2	GROUP 3	3 GROUP	4	
4 UE	—— Л.T.	4 040E 12	4 141E 13	2 700E 11			
1 HE		4.840E-13					
2 AB: 4 TO		6.273E-02 9.122E-01					
5 IN		5.052E-01					
6	O101	0.000E+00					
7		0.000E+00					
8		0.000E+00					
9		0.000E+00					
-		0.00000				00	

0.000E+00

0.000E+00

0.000E+00

0.000E+00 ...

0.000E+00

0.000E+00

10

11

0.000E+00

0.000E+00

```
12
           0.000E+00 0.000E+00 0.000E+00
                                          0.000E+00
 13
                                          0.000E+00 ...
           0.000E+00 0.000E+00 0.000E+00
** CARBON P1 **
                                GROUP 3 GROUP 4
           GROUP 1 GROUP 2
POSITION
  5 INGRP
          -3.595E-03
                     1.509E-02 5.007E-02 4.900E-02
           0.000E+00 1.685E-01 1.122E-01 3.592E-02 ...
  7
           0.000E+00 0.000E+00 -1.072E-02 -5.070E-02
                                         3.419E-02 ...
  8
           0.000E+00 0.000E+00 0.000E+00
  9
           10
           0.000E+00 0.000E+00 0.000E+00 0.000E+00
           0.000E+00 0.000E+00 0.000E+00 0.000E+00
 11
 12
           0.000E+00 0.000E+00 0.000E+00 0.000E+00
 13
           0.000E+00 0.000E+00 0.000E+00 0.000E+00 ...
. . .
** TUNGST PO **
POSITION
           GROUP 1 GROUP 2
                                GROUP 3
                                          GROUP 4
_____
           _____
                     _____
                               _____
                                          _____
  1 HEAT
           7.722E-14 6.395E-14 5.750E-14
                                         5.285E-14 ...
  2 ABS
          -2.338E+00 -2.016E+00 -1.918E+00 -1.660E+00
                                         3.139E+00
  4 TOTAL
           2.778E+00 2.888E+00 2.982E+00
  5 INGRP
           4.152E-01 5.876E-01 7.029E-01 8.825E-01 ...
  6
           0.000E+00 9.812E-02 5.632E-02 6.523E-02 ...
  7
           0.000E+00 0.000E+00
                               2.114E-02 3.397E-02
  8
           0.000E+00 0.000E+00 0.000E+00 5.000E-02
  9
           0.000E+00 0.000E+00 0.000E+00 0.000E+00
           10
          0.000E+00 0.000E+00 0.000E+00 0.000E+00
 11
TRANSX COMPLETE
                                                         2.3S
Sample CARD Output
CARBON PO 34X 30 TABLE
                                                                  0
4.84046E-13 6.27289E-02 0.00000E+00 9.12203E-01 5.05172E-02 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                   2
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                   3
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                   4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                   5
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 4.14145E-13 6.84320E-02
                                                                   6
```

0.00000E+00 8.80773E-01 5.84583E-02 2.61000E-01 0.00000E+00 0.00000E+00

0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00

7

8

```
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            9
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            10
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            11
0.00000E+00 0.00000E+00 3.71959E-13 8.89298E-02 0.00000E+00 9.02727E-01
                                                                            12
1.13132E-01 1.89513E-01 8.68378E-02 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            13
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            14
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            15
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            16
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            17
2.64774E-13 9.78256E-02 0.00000E+00 8.61282E-01 1.25263E-01 2.33726E-01
                                                                            18
1.39455E-01 1.20101E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            19
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            20
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            21
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            22
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 2.12741E-13 1.40423E-01
                                                                           23
0.00000E+00 9.23660E-01 9.45104E-02 2.17309E-01 1.53811E-01 1.26440E-01
                                                                            24
5.05288E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            25
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            26
CARBON P1 34X 30 TABLE
                                                                            0
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00-3.59481E-03 0.00000E+00
                                                                             1
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             2
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             3
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             4
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             5
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             6
0.00000E+00 0.00000E+00 1.50855E-02 1.68473E-01 0.00000E+00 0.00000E+00
                                                                             7
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             8
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            9
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            10
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            11
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            12
5.00742E-02 1.12206E-01-1.07248E-02 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            13
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            14
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            15
TUNGST PO 34X 30 TABLE
                                                                             0
7.72240E-14-2.33829E+00 0.00000E+00 2.77838E+00 4.15159E-01 0.00000E+00
                                                                             1
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             2
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             3
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             5
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 6.39486E-14-2.01584E+00
                                                                             6
0.00000E+00 2.88828E+00 5.87563E-01 9.81161E-02 0.00000E+00 0.00000E+00
                                                                             7
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                             8
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            9
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            10
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            11
0.00000E+00 0.00000E+00 5.75040E-14-1.91808E+00 0.00000E+00 2.98227E+00
                                                                            12
7.02909E-01 5.63160E-02 2.11383E-02 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            13
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            14
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
                                                                            15
```

## Sample Problem 2

The following selected parts of the output for Sample Problem 2 show the main differences between group-ordered output and material-ordered output. The ellipses show where portions of the output have been removed to make it fit on the page better.

. . .

# GROUP-ORDERED CROSS SECTION TABLES

WORDS AVAILABLE FOR TABLE =293235 NUMBER OF GROUPS PER PASS = 30

0.2S

** GROUP	1 **			
POSITION	CARBON PO	CARBON P1	TUNGST PO	TUNGST P1
1 HEAT	4.840E-13	0.000E+00	7.722E-14	0.000E+00
2 ABS	6.273E-02	0.000E+00	-2.338E+00	0.000E+00
3 NUSIGF	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4 TOTAL	9.122E-01	0.000E+00	2.778E+00	0.000E+00
5 INGRP	5.052E-02	-3.595E-03	4.152E-01	1.063E-01
** GROUP 2	2 **			
POSITION	CARBON PO	CARBON P1	TUNGST PO	TUNGST P1
1 HEAT	4.141E-13	0.000E+00	6.395E-14	0.000E+00
2 ABS	6.843E-02	0.000E+00	-2.016E+00	0.000E+00
3 NUSIGF	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4 TOTAL	8.808E-01	0.000E+00	2.888E+00	0.000E+00
5 INGRP	5.846E-02	1.509E-02	5.876E-01	1.958E-01
6	2.610E-01	1.685E-01	9.812E-02	3.083E-02
** GROUP	3 **			
POSITION	CARBON PO	CARBON P1	TUNGST PO	TUNGST P1
1 HEAT	3.720E-13	0.000E+00	5.750E-14	0.000E+00
2 ABS	8.893E-02	0.000E+00	-1.918E+00	0.000E+00
3 NUSIGF	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4 TOTAL	9.027E-01	0.000E+00	2.982E+00	0.000E+00
5 INGRP	1.131E-01	5.007E-02	7.029E-01	2.382E-01
6	1.895E-01	1.122E-01	5.632E-02	1.033E-02
7	8.684E-02	-1.072E-02	2.114E-02	3.049E-03
	_			

\*\* GROUP 4 \*\*

POSITION	CARBON PO	CARBON P1	TUNGST PO	TUNGST P1	
1 HEAT	2.648E-13	0.000E+00	5.285E-14	0.000E+00	
2 ABS	9.783E-02	0.000E+00	-1.660E+00	0.000E+00	
3 NUSIGF	0.000E+00	0.000E+00	0.000E+00	0.000E+00	
4 TOTAL	8.613E-01	0.000E+00	3.139E+00	0.000E+00	
5 INGRP	1.253E-01	4.900E-02	8.825E-01	2.986E-01	
6	2.337E-01	3.592E-02	6.523E-02	1.405E-02	
7	1.395E-01	-5.070E-02	3.397E-02	4.507E-03	
8	1.201E-01	3.419E-02	5.000E-02	7.066E-03	

. . . .

## Sample FIDO Output

This is a portion of the FIDO file produced by Sample Problem 3. Note the use of the repeat option (R) to reduce the number of zeros in the file. Also note that each section of the table is terminated (T).

AL-27 PO 462	K 42 TABLE					0
4853214+0	-125011-5	0+0	1370380-6	1351485-74	1R 0+0	1
4782239+0	-131070-5	0+0	1376950-6	1345390-7	1579228-7	2
40R 0+0	4172989+0	-137062-5	0+0	1381834-6	1905284-7	3
1645197-7	4424464-839R	0+0	3024617+0	-145317-5	0+0	4
1372002-6	2143598-7	1436255-7	6515701-8	4029540-838	BR 0+0	5
1525512+0	-136368-5	0+0	1347490-6	2446186-7	1603739-7	6
7063104-8	5850607-8	7195758 <b>–</b> 83'	7R 0+0	5759916-1	-122417-5	7
0+0	1434578-6	3622383-7	2225031-7	8017632-8	7599577-8	8
8982142-8	8102238-836R	0+0	4084915-1	-883606-6	0+0	9
1744504-6	8556168-7	4623703-7	1966109-7	1720993-7	1862897-7	10
1666533-7	1343128-735R	0+0	3420562-1	-638749-6	0+0	11
2028878-6	1046921-6	3246706-7	1474077-7	9130573-8	8814702-8	12
8281922 <del>-</del> 8	7893734-8	8470646-83	4R 0+0	287 <b>4</b> 572 <b>-</b> 1	-364922-6	13
0+0	2313129-6	1 <b>4</b> 8938 <b>4-</b> 6	4769129-7	1361422-7	78 <b>4</b> 7955 <b>-</b> 8	14
8011077 <del>-</del> 8	8681245-8	8326775-8	8076120-8	8362688-83	3R 0+0	15
2669560-1	-307740-6	0+0	2559229-6	1725468-6	4832581-7	16
1849300-7	8692349-8	7190167-8	771 <b>4</b> 827 <b>-</b> 8	8330074-8	7761373-8	17
7435174-8	9456518-832R	0+0	2172306-1	-250957-6	0+0	18
2720071-6	1886117-6	5327229-7	1461140-7	2712 <del>444-</del> 8	1036958-7	19
67617 <b>4</b> 5 <b>-</b> 8	7046503-8	7275467-8	6538448-8	6289563-8	7994376-8	20
• • •						
194298-10	773477-10	180186 <b>-</b> 09	294745-09	341299-09	610631-09	148
3984604-9	T					149
AL-27 P1 46	3X 42 TABLE					0
4R 0+0	7017552 <del>-</del> 845R	0+0	8125679-8	4661935-844	4R 0+0	1
9478804-8	2160393-8	7284464-94	3R 0+0	8426757-8	1164833-8	2
1679947-8	1781045 <b>-</b> 942R	0+0	7731200-8	1291785-8	7735120-9	3
35775 <b>47-</b> 9	7805440-941R	0+0	1032406-7	3047906-9	4103804-9	4
8116636-9	8614968-9	1438678-94	OR 0+0	3001110-7	5313086-9	5
1238474-8	1287040-8	9870019-9	5948243-9	1102423-839	9R 0+0	6
4193276-7	3225548-8	2574680-9	4200667-9	535238 <b>4-</b> 9	5787241-9	7
7521997-9	7063515 <del>-</del> 938R	0+0	6207061-7	4131107-9	2515195 <b>-</b> 9	8

```
-147460-8 3856838-9 6351238-9 6564295-9 6115635-9 4125447-9 9 ...
1187430-8 -258527-640R 0+0 T 66
```

Complete output listings from all the sample problems are available in the  ${\it TRANSX}$  2.0 distribution package.

## Appendix B. MATXS FILE DESCRIPTION

The following description of the MATXS format uses the standard CCCC form. It was copied from the comment cards at the start of the MATXSR module of NJOY 91.0.

	************	*******	<b>*</b> *
С	PROPOSED 09/09/77		-
С	(MODIFIED 09/80)		_
C	(NOMENCLATURE CHANGED OF	3/88)	_
C	(MODIFIED FOR CONST SUB-	-BLOCKS 06/90)	_
С	(ORDERING CHANGED 10/90)	)	_
С			_
CF	MATXS		_
CE	MATERIAL CROSS SECTION FILE		_
С			_
CN	THIS FILE CONTAINS CROS	SS SECTION	_
CN	VECTORS AND MATRICES FO		_
CN	PARTICLES, MATERIALS, A		_
CN	DELAYED NEUTRON SPECTRA	·	
CN	AND DECAY HEAT AND PHOT	•	
CN	AND DECAI REAL AND PROD	IUM SPECIKA.	
-	CODMATC CIVEN AND COD CITE EVOUANCE	CONTY	_
CN	FORMATS GIVEN ARE FOR FILE EXCHANGE	- UNLY	
C			
•	***************	********	ሾሞ
C			
C			
C			
CS	FILE STRUCTURE		_
CS			-
CS	RECORD TYPE		
		PRESENT IF	-
CS			-
CS	FILE IDENTIFICATION		- - -
CS CS	FILE IDENTIFICATION FILE CONTROL	=======================================	- - -
CS	FILE IDENTIFICATION	ALWAYS	- - - -
CS CS	FILE IDENTIFICATION FILE CONTROL	ALWAYS ALWAYS	- - - -
CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION	ALWAYS ALWAYS ALWAYS	- - - - -
CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION	ALWAYS ALWAYS ALWAYS	
CS CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA	ALWAYS ALWAYS ALWAYS	- - - - - -
CS CS CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	- - - - - -
CS CS CS CS CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  *************(REPEAT FOR ALL PARTICLES) * GROUP STRUCTURES	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS CS CS CS CS CS CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **************(REPEAT FOR ALL PARTICLES)  * GROUP STRUCTURES  ***********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS CS CS CS CS CS CS CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **************(REPEAT FOR ALL PARTICLES)  * GROUP STRUCTURES  ***********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  ***************(REPEAT FOR ALL PARTICLES) * GROUP STRUCTURES  ****************  *****************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS C	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS C	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS C	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS C	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS C	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS  ALWAYS  ALWAYS	
CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS	
CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  ****************  GROUP STRUCTURES  ************  ***********  *********	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS  ALWAYS  ALWAYS	
CS	FILE IDENTIFICATION FILE CONTROL SET HOLLERITH IDENTIFICATION FILE DATA  **********************************	ALWAYS ALWAYS ALWAYS ALWAYS ALWAYS  ALWAYS  ALWAYS  N1DB.GT.O	

```
N2D.GT.O
CS
    * * * MATRIX CONTROL
CS
CS
    * * * ******(REPEAT FOR ALL SUB-BLOCKS)
    * * * * MATRIX SUB-BLOCK
CS
                                              N2D.GT.O
    * * * *****
CS
    * * *
    * * * CONSTANT SUB-BLOCK
                                     JCONST.GT.O
CS
CS
    * * *
    *****
CR.
          FILE IDENTIFICATION
С
CL HNAME, (HUSE(I), I=1,2), IVERS
С
CW 1+3*MULT
CB FORMAT(4H OV ,A8,1H*,2A8,1H*,I6)
CD HNAME HOLLERITH FILE NAME - MATXS - (A8)
CD HUSE HOLLERITH USER IDENTIFIATION (A8)
CD IVERS
                FILE VERSION NUMBER
               DOUBLE PRECISION PARAMETER
                     1- A8 WORD IS SINGLE WORD
CD
CD
                      2- A8 WORD IS DOUBLE PRECISION WORD
C
CR
          FILE CONTROL
С
CL
   NPART, NTYPE, NHOLL, NMAT, MAXW, LENGTH
С
CW
С
CB
    FORMAT(4H 1D ,4I6)
С
CD NPART NUMBER OF PARTICLES FOR WHICH GROUP
                 STRUCTURES ARE GIVEN
    NTYPE NUMBER OF DATA TYPES PRESENT IN SET NHOLL NUMBER OF WORDS IN SET HOLLERITH
CD
CD
CD
                    IDENTIFICATION RECORD
CD NMAT NUMBER OF MATERIALS ON FILE
CD MAXW
              MAXIMUM RECORD SIZE FOR SUB-BLOCKING
CD LENGTH
              LENGTH OF FILE
С
С
```

```
CR
           SET HOLLERITH IDENTIFICATION
С
CL
     (HSETID(I), I=1, NHOLL)
С
CW
     NHOLL*MULT
С
CB
     FORMAT(4H 2D ,8A8/(9A8))
С
     HSETID HOLLERITH IDENTIFICATION OF SET (A8)
CD
CD
               (TO BE EDITED OUT 72 CHARACTERS PER LINE)
C
C
C
CR
         FILE DATA
С
CL
     (HPRT(J), J=1, NPART), (HTYPE(K), K=1, NTYPE), (HMATN(I), I=1, NMAT),
    1(NGRP(J), J=1, NPART), (JINP(K), K=1, NTYPE, (JOUTP(K), K=1, NTYPE),
CL
CL
    2(NSUBM(I)I=1,NMAT),(LOCM(I),I=1,NMAT)
С
CW
     (NPART+NTYPE+NMAT)*MULT+2*NTYPE+NPART+2*NMAT
С
     FORMAT(4H 3D ,8A8/(9A8)) HPRT,HTYPE,HMATN
CB
CB
     FORMAT(12I6)
                              NGRP, JINP, JOUTP, NSUBM, LOCM
С
CD
     HPRT(J) HOLLERITH IDENTIFICATION FOR PARTICLE J
CD
                  N NEUTRON
CD
                    G
                             GAMMA
                    Ρ
CD
                             PROTON
CD
                    D
                             DEUTERON
CD
                    Т
                            TRITON
                           HE-3 NUCLEUS
CD
                    H
CD
                             ALPHA (HE-4 NUCLEUS)
                    Α
CD
                    В
                             BETA
CD
                             RESIDUAL OR RECOIL
                             (HEAVIER THAN ALPHA)
CD
CD
     HTYPE(K) HOLLERITH IDENTIFICATION FOR DATA TYPE K
                    NSCAT
CD
                             NEUTRON SCATTERING
CD
                    NG
                             NEUTRON INDUCED GAMMA PRODUCTION
CD
                    GSCAT
                             GAMMA SCATTERING
CD
                    PN
                             PROTON INDUCED NEUTRON PRODUCTION
CD
CD
CD
                    DKN
                             DELAYED NEUTRON DATA
CD
                             DECAY HEAT AND GAMMA DATA
CD
                    DKHG
CD
                    DKB
                            DECAY BETA DATA
     HMATN(I) HOLLERITH IDENTIFICATION FOR MATERIAL I
CD
     NGRP(J)
CD
               NUMBER OF ENERGY GROUPS FOR PARTICLE J
CD
     JINP(K)
                TYPE OF INCIDENT PARTICLE ASSOCIATED WITH
CD
                 DATA TYPE K. FOR DK DATA TYPES, JINP IS O.
```

```
CD
     JOUTP(K) TYPE OF OUTGOING PARTICLE ASSOCIATED WITH
CD
                 DATA TYPE K
     NSUBM(I) NUMBER OF SUBMATERIALS FOR MATERIAL I
CD
CD
     LOCM(I)
               LOCATION OF MATERIAL I
С
C
CR
           GROUP STRUCTURE
С
CL
   (GPB(I),I=1,NGR),EMIN
C
CC
    NGR=NGRP(J)
C
CW
     NGRP(J)+1
С
     FORMAT(4H 4D ,1P5E12.5/(6E12.5))
CB
С
     GPB(I) MAXIMUM ENERGY BOUND FOR GROUP I FOR PARTICLE J
EMIN MINIMUM ENERGY BOUND FOR PARTICLE J
CD
CD
C
CR
          MATERIAL CONTROL
С
     HMAT, AMASS, (TEMP(I), SIGZ(I), ITYPE(I), N1D(I), N2D(I),
CL
CL
    1LOCS(I), I=1, NSUBM)
С
CW
    MULT+1+6*NSUBM
С
     FORMAT(4H 6D ,A8,1H*,1P2E12.5/(2E12.5,5I6))
CB
С
CD
     TAMH
                HOLLERITH MATERIAL IDENTIFIER
CD
     AMASS
              ATOMIC WEIGHT RATIO
CD
     TEMP
                AMBIENT TEMPERATURE OR OTHER PARAMETERS FOR
CD
                    SUBMATERIAL I
     SIGZ
CD
                DILUTION FACTOR OR OTHER PARAMETERS FOR
CD
                    SUBMATERIAL I
CD
     ITYPE
                DATA TYPE FOR SUBMATERIAL I
     N1D
CD
                NUMBER OF VECTORS FOR SUBMATERIAL I
CD
     N2D
                NUMBER OF MATRIX BLOCKS FOR SUBMATERIAL I
     LOCS LOCATION OF SUBMATERIAL I
CD
С
С
C
C-----
CR
         VECTOR CONTROL
С
CL
     (HVPS(I),I=1,N1D),(NFG(I),I=1,N1D),(NLG(I),I=1,N1D)
```

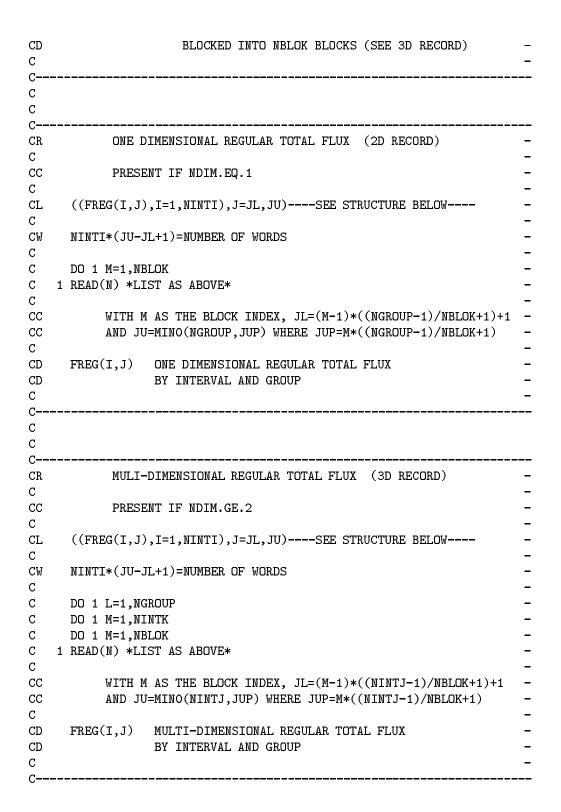
```
С
CW
     (MULT+2)*N1D
С
CB
     FORMAT(4H 7D ,8A8/(9A8))
                                   HVPS
CB
     FORMAT(12I6)
                                    IBLK,NFG,NLG
С
     HVPS(I) HOLLERITH IDENTIFIER OF VECTOR
CD
CD
                       NELAS
                                NEUTRON ELASTIC SCATTERING
                       N2N
CD
                                (N,2N)
CD
                       NNF
                               SECOND CHANCE FISSION
CD
                       GABS
                               GAMMA ABSORPTION
CD
                      P2N
                               PROTONS IN, 2 NEUTRONS OUT
CD
CD
CD
   NFG(I) NUMBER OF FIRST GROUP IN BAND FOR VECTOR I NLG(I) NUMBER OF LAST GROUP IN BAND FOR VECTOR I
CD
CD
С
С
С
C----
CR
          VECTOR BLOCK
С
CL
     (VPS(I), I=1, KMAX)
C
CC
     KMAX=SUM OVER GROUP BAND FOR EACH VECTOR IN BLOCK J
CW
     KMAX
С
CB
     FORMAT(4H 8D ,1P5E12.5/(6E12.5))
C
CD
     VPS(I)
                 DATA FOR GROUP BANDS FOR VECTORS IN BLOCK J.
CD
                 BLOCK SIZE IS DETERMINED BY TAKING ALL THE GROUP
CD
                 BANDS THAT HAVE A TOTAL LENGTH LESS THAN OR EQUAL
CD
                 TO MAXW.
С
C
CR
        SCATTERING MATRIX CONTROL
CL
     HMTX,LORD,JCONST,
CL
    1(JBAND(L),L=1,NOUTG(K)),(IJJ(L),L=1,NOUTG(K))
С
CW
     MULT+2+2*NOUTG(K)
С
     FORMAT(4H 9D ,A8/(12I6))
                                   HMTX,LORD,JCONST,
CB
CB
                                     JBAND,IJJ
С
CD
     HMTX
                HOLLERITH IDENTIFICATION OF BLOCK
CD
     LORD
                 NUMBER OF ORDERS PRESENT
```

CD CD	JCONST JBAND(L)	NUMBER OF GROUPS WITH CONSTANT SPECTRUM BANDWIDTH FOR GROUP L	- -
CD C	IJJ(L)	LOWEST GROUP IN BAND FOR GROUP L	<del>-</del>
C			
C			
CR	SCATT	TERING SUB-BLOCK	_
C CL	(SCAT(K),K=	-1 KMAY)	_
C	(BOH1 (II), III-	1, min x)	_
CC	KMAX=LORD T	TIMES THE SUM OVER ALL JBAND IN THE GROUP RANGE OF	_
CC	THI	S SUB-BLOCK	_
C			-
CB	FORMAT(5H 1	OD ,1P5E12.5/(6E12.5))	_
C CW	KMAX		_
C	MIAX		_
CD	SCAT(K)	MATRIX DATA GIVEN AS BANDS OF ELEMENTS FOR INITIAL	_
CD		GROUPS THAT LEAD TO EACH FINAL GROUP. THE ORDER	_
CD		OF THE ELEMENTS IS AS FOLLOWS: BAND FOR PO OF	-
CD		GROUP I, BAND FOR P1 OF GROUP I,, BAND FOR PO	_
CD		OF GROUP I+1, BAND FOR P1 OF GROUP I+1, ETC. THE	-
CD CD		GROUPS IN EACH BAND ARE GIVEN IN DESCENDING ORDER.  THE SIZE OF EACH SUB-BLOCK IS DETERMINED BY THE	_
CD		TOTAL LENGTH OF A GROUP OF BANDS THAT IS LESS THAN	_
CD		OR EQUAL TO MAXW.	_
CD			_
CD		IF JCONST.GT.O, THE CONTRIBUTIONS FROM THE JCONST	_
CD		LOW-ENERGY GROUPS ARE GIVEN SEPARATELY.	_
C			_
C			
C			_
C			
CR	CONST	CANT SUB-BLOCK	_
C	(2222(1) 1	( NOVE (V) ) (DD OD (T) T T ( NTV (V))	_
CL C	(SPEC(L),L=	=1,NOUTG(K)),(PROD(L),L=L1,NING(K))	_
CC	L1=NING(K)-	- ICONST+1	_
C	LI-WING(II)	300165111	_
CW	NOUTG(K)+JC	CONST	_
С			-
CB	FORMAT(4H11	D ,1P5E12.5/(6E12.5))	-
C			-
CD	SPEC	NORMALIZED SPECTRUM OF FINAL PARTICLES FOR INITIAL	-
CD CD	PROD	PARTICLES IN GROUPS L1 TO NING(K) PRODUCTION CROSS SECTION (E.G., NU*SIGF) FOR	_
CD	FRUD	INITIAL GROUPS L1 THROUGH NING(K)	_
CD		where II impound the contraction	_
CD	THIS C	PTION IS NORMALLY USED FOR THE ENERGY-INDEPENDENT	_
CD	NEUTRO	ON AND PHOTON SPECTRA FROM FISSION AND RADIATIVE	-

## Appendix C. RTFLUX FILE DESCRIPTION

The following description of the RTFLUX format uses the standard CCCC form. These lines were copied from the CCCC-IV reference.

C****	*****	·*************************************	****
С		REVISED 11/30/76	_
С			_
CF	RTFI	LUX-IV	_
CE		JLAR TOTAL FLUXES	_
C	шас	JUNIO TOTALI TUVALO	_
·	***	*******************	****
C			1111.
C			
•			
C	TTT 1	TDENTITECATION	
CR C	LILI	IDENTIFICATION	_
•	IINI AMEL (IIIIGI	1/T) T 4 0) TUDDG	_
CL	HNAME, (HUSE	E(I),I=1,2),IVERS	_
C			_
CW	1+3*MULT		_
С		, ,	_
CD	HNAME	HOLLERITH FILE NAME - RTFLUX - (A6)	_
CD	HUSE	HOLLERITH USER IDENTIFICATION (A6)	_
CD	IVERS	FILE VERSION NUMBER	_
CD	MULT	DOUBLE PRECISION PARAMETER	_
CD		1- A6 WORD IS SINGLE WORD	_
CD		2- A6 WORD IS DOUBLE PRECISION WORD	_
С			_
C			
С			
С			
C			
CR	SPEC	CIFICATIONS (1D RECORD)	_
С			_
CL	NDIM, NGROUE	P, NINTI, NINTJ, NINTK, ITER, EFFK, POWER, NBLOK	_
С	·		_
CW	9=NUMBER OF	WORDS	_
C			_
CD	NDIM	NUMBER OF DIMENSIONS	_
CD	NGROUP	NUMBER OF ENERGY GROUPS	_
CD	NINTI	NUMBER OF FIRST DIMENSION FINE MESH INTERVALS	
CD	NINTJ	NUMBER OF SECOND DIMENSION FINE MESH INTERVALS	_
CD	NINIO	NINTJ.EQ.1 IF NDIM.EQ.1	_
CD	אידוא דוא	NUMBER OF THIRD DIMENSION INTERVALS	_
CD	NINTK	NINTK.EQ.1 IF NDIM.LE.2	_
	ITER	·	_
CD		OUTER ITERATION NUMBER AT WHICH FLUX WAS WRITTEN	_
CD	EFFK	EFFECTIVE MULTIPLICATION FACTOR	_
CD	POWER	POWER IN WATTS TO WHICH FLUX IS NORMALIZED	_
CD	NBLOK	DATA BLOCKING FACTOR	-
CD		IF NDIM.EQ.1, THE GROUP VARIABLE IS BLOCKED	_
CD		INTO NBLOK BLOCKS (SEE 2D RECORD BELOW)	_
CD		IF NDIM.GE.2, THE 2ND DIMENSION VARIABLE IS	_



## Appendix D. RZFLUX FILE DESCRIPTION

The following description of the RZFLUX format uses the standard CCCC form. These lines were copied from the CCCC-IV reference.

C***	*******	***************************************	***
C		REVISED 11/30/76	_
C		11/30/10	_
	DG	עד עון זרדע	
CF		#FLUX-IV	_
CE	RE	EGULAR ZONE FLUX BY GROUP, AVERAGED OVER EACH ZONE	_
С			-
C***	******	******************	***
С			
С			
C			
CR	FI	LE IDENTIFICATION	_
С			_
CL	ниме (ні	JSE(I), I=1,2), IVERS	_
C	IIIIAIIL, (IIC	701(1),1-1,2),111110	_
_	4 . 2		_
CW	1+3*MULT		_
C			_
CD	HNAME	HOLLERITH FILE NAME - RZFLUX - (A6)	-
CD	HUSE	HOLLERITH USER IDENTIFICATION (A6)	-
$^{\rm CD}$	IVERS	FILE VERSION NUMBER	-
CD	MULT	DOUBLE PRECISION PARAMETER	-
CD		1- A6 WORD IS SINGLE WORD	-
CD		2- A6 WORD IS DOUBLE PRECISION WORD	_
С			_
C			
C			
C			
C			
CR	SE	PECIFICATIONS (1D RECORD)	_
C	DI.	LOTI TONITIONS (ID IMPOSID)	_
CL	TIME DOME	ER, VOL, EFFK, EIVS, DKDS, TNL, TNA, TNSL, TNBL, TNBAL, TNCRA,	_
	•		_
CL	1(X(1),1-1	1,3),NBLOK,ITPS,NZONE,NGROUP,NCY	_
C			-
CW	20=NUMBER	R OF WORDS	_
С			_
CD	TIME	REFERENCE REAL TIME, DAYS	-
CD	POWER	POWER LEVEL FOR ACTUAL NEUTRONICS PROBLEM,	_
CD		WATTS TERMAL	_
CD	VOL	VOLUME OVER WHICH POWER WAS DETERMINED, CC	_
CD	EFFK	EFFECTIVE MULTIPLICATION FACTOR	-
CD	EIVS	EIGENVALUE OF SEARCH PROBLEM	_
CD	DKDS	DERIVATIVE OF SEARCH PROBLEM	_
CD	TNL	TOTAL NEUTRON LOSSES	_
CD	TNA	TOTAL NEUTRON ABSORPTIONS	_
			_
CD	TNSL	TOTAL NEUTRON SURFACE LEAKAGE TOTAL NEUTRON BUCKLING LOSS	_
O.D.		TOTAL MEDITRIM ROTERTING TINGS	_
CD	TNBL		
CD CD	TNBL TNBAL TNCRA	TOTAL NEUTRON BLACK ABSORBER LOSS TOTAL NEUTRON CONTROL ROD ABSORPTIONS	_

CD CD	X(I),I=1,3 NBLOK	RESERVED DATA BLOCKING FACTOR. THE GEOMETRIC ZONE VARIABLE IS BLOCKED INTO NBLOK BLOCKS.	- - -
CD CD CD CD CD	ITPS NZONE	ITERATIVE PROCESS STATE  =0, NO ITERATIONS DONE  =1, CONVERGENCE SATISFIED  =2, NOT CONVERGED, BUT CONVERGING  =3, NOT CONVERGED, NOT CONVERGING  NUMBER OF GEOMETRIC ZONES	- - - -
CD CD	NGROUP NCY	NUMBER OF ENERGY GROUPS	- - -
C C C C			
CR C	FLUX	VALUES (2D RECORD)	-
CL C	((ZGF(K,J),	K=1,NGROUP),J=JL,JU)SEE STRUCTURE BELOW	_
CW C	NGROUP*(JU-	-JL+1)=NUMBER OF WORDS	-
С С С	DO 1 M=1,NE 1 READ(N) *LI	ST AS ABOVE*	- - -
CC CC		M AS THE BLOCK INDEX, JL=(M-1)*((NZONE-1)/NBLOK+1)+1 U=MINO(NZONE, JUP) WHERE JUP=M*((NZONE-1)/NBLOK+1)	- - -
CD C	ZGF(K,J)	REGULAR ZONE FLUX BY GROUP, AVERAGED OVER ZONE. NEUTRONS/SEC-CM**2.	- - -

## Appendix E. RZMFLX FILE DESCRIPTION

The following description of the RZMFLX format uses the standard CCCC form.

C****	******	******************
С		PROPOSED -
C		- · · · · · · · · · · · · · · · · · · ·
CF	R7ME	LX-IV -
CE		LAR ZONE-AVERAGED MOMENTS FLUX
	REGU	LAR ZUNE-AVERAGED MUMENIS FLUA
C		-
•	*****	*****************
C		
С		
C		
CR	FILE	IDENTIFICATION -
С		-
CL	HNAME, (HUSE	(I),I=1,2),IVERS -
С		<del>-</del>
CW	1+3*MULT	<del>-</del>
С		<del>-</del>
CD	HNAME	HOLLERITH FILE NAME - RZMFLX - (A6) -
CD	HUSE	HOLLERITH USER IDENTIFICATION (A6) -
CD	IVERS	FILE VERSION NUMBER -
CD	MULT	DOUBLE PRECISION PARAMETER -
CD		1- A8 WORD IS SINGLE WORD -
CD		2- A8 WORD IS DOUBLE PRECISION WORD -
C		-
C		
Ċ		
C		
C		
CR	SPEC	IFICATIONS -
C	21 _ 3	
CL	NDTM.NGROUP	,NINTI,NINTJ,NINTK,NORD,EFFK,POWER -
C	110111,11010001	
CW	8=NUMBER OF	LIORNS -
C	O-NOMBER OF	words –
CD	NDIM	NUMBER OF DIMENSIONS -
CD	NGROUP	NUMBER OF GROUPS -
CD	NINTI	NUMBER OF FIRST DIMENSION INTERVALS -
CD	NINTJ	NUMBER OF SECOND DIMENSION INTERVALS -
CD		NINTJ.EQ.1 IF NDIM.EQ.1
CD	NINTK	NUMBER OF THIRD DIMENSION INTERVALS -
CD		NINTK.EQ.1 IF NDIM.LE.2
CD	NORD	NUMBER OF LEGENDRE MOMENTS -
CD	EFFK	EFFECTIVE MULTIPLICATION FACTOR -
CD	POWER	POWER IN WATTS TO WHICH FLUX IS NORMALIZED -
C		-
C		
C		
С		

C		
CR CR	REGULAR MOMENTS FLUXES ON MULTIDIMENSIONAL INTERVALS	_
C CL	((FLUX(M,I),M=1,NORD,I=1,NINTI)NOTE STRUCTURE BELOW	_
C		-
CW C	NORD*NINTI=NUMBER OF WORDS	-
C		_

## Appendix F. ISOTXS FILE DESCRIPTION

The following description of the ISOTXS format uses the standard CCCC form. It was copied from the CCCC-IV report.  $^{25}\,$ 

C***	****	*************	********	**
C		REVISED 11/30/76		_
С				-
CF		ISOTXS-IV		_
CE		MICROSCOPIC GROUP NEUTRON CROSS SEC	CTIONS	_
C				_
CN		THIS FILE PROVIDES A BA	ASTC BROAD GROUP	_
CN		LIBRARY, ORDERED BY ISO		_
C		LIBITARII, ORDERED DI 150	JIOI E.	
CN		FORMATS GIVEN ARE FOR FILE EXCHANGE	ONIV	
CN		FURMAIS GIVEN ARE FUR FILE EXCHANGE	S ONL!	
•				_
•	****	<*************************************	********	**
С				
С				
C				
CS		FILE STRUCTURE		-
CS				-
CS		RECORD TYPE	PRESENT IF	_
CS			=======================================	_
CS		FILE IDENTIFICATION	ALWAYS	_
CS		FILE CONTROL	ALWAYS	_
CS		FILE DATA	ALWAYS	_
CS		FILE-WIDE CHI DATA	ICHIST.GT.1	_
CS				_
CS	****	*********(REPEAT FOR ALL ISOTOPES)		_
CS	*	ISOTOPE CONTROL AND GROUP		_
CS	*	INDEPENDENT DATA	ATHAVC	_
		PRINCIPAL CROSS SECTIONS		
CS	*		ALWAYS	
CS	*	ISOTOPE CHI DATA	ICHI.GT.1	_
0.0	*	/		_
		**************************************	BLOCKS)	-
	* *	* *******(REPEAT FROM 1 TO NSBLOK)		_
CS	* *	* * SCATTERING SUB-BLOCK	LORDN(N).GT.O	-
CS	***	******		-
С				_
C				
С				
С				
C				
CR		FILE IDENTIFICATION		_
C				_
CL	HN A	ME,(HUSE(I),I=1,2),IVERS		_
C	111/1	, (		_
CW	415	*MULT		_
	1+3	PTIUL1		_
C	TO *	MATERIAL ON AC ALL TO		_
CB	FUF	MAT(4H OV ,A8,1H*,2A6,1H*,I6)		_
С				_

```
CD
                   HOLLERITH FILE NAME - MATXS - (A8)
      {\sf HNAME}
CD
      HUSE
                   HOLLERITH USER IDENTIFIATION
                                                    (8A)
CD
      IVERS
                  FILE VERSION NUMBER
CD
     MULT
                   DOUBLE PRECISION PARAMETER
CD
                        1- A6 WORD IS SINGLE WORD
CD
                        2- A6 WORD IS DOUBLE PRECISION WORD
C
CR
            FILE CONTROL (1D RECORD)
C
CL
      NGROUP, NISO, MAXUP, MAXDN, MAXORD, ICHIST, NSCMAX, NSBLOK
C
CW
      8=NUMBER OF WORDS
C
CB
     FORMAT(4H 1D ,4I6)
С
CD
      NGROUP
                 NUMBER OF ENERGY GROUPS IN FILE
CD
     NISO
                 NUMBER OF ISOTOPES IN FILE
CD
     MAXUP
                 MAXIMUM NUMBER OF UPSCATTER GROUPS
     MAXDN
MAXORD
CD
                 MAXIMUM NUMBER OF DOWNSCATTER GROUPS
CD
                 MAXIMUM SCATTERING ORDER (MAXIMUM VALUE OF
                    LEGENDRE EXPANSION INDEX USED IN FILE).
CD
CD
      ICHIST
                 FILE-WIDE FISSION SPECTRUM FLAG
CD
                    ICHIST.EQ.O NO FILE-WIDE SPECTRUM
CD
                    ICHIST.EQ.1
                                   FILE-WIDE CHI VECTOR
CD
                    ICHIST.GT.1 FILE-WIDE CHI MATRIX
CD
                 MAIMUM NUMBER OF BLOCKS OF SCATTERING DATA
     NSCMAX
CD
      NSBLOK
                 SUBBLOCKING CONTROL FOR SCATTER MATRICES. THE
CD
                    SCATTERING DATA ARE SUBBLOCKED INTO NSBLOK
CD
                    RECORDS(SUBBLOCKS) PER SCATTERING BLOCK.
С
С
С
C---
CR
           FILE DATA
C
CL
      (HSETID(I), I=1,12), (HISONM(I), I=1, NISO),
     1(CHI(J), J=1, NGROUP), (VEL(J), J=1, NGROUP,
CL
CL
     2(EMAX(J), J=1, NGROUP), EMIN, (LOCA(I), I=1, NISO)
С
CW
      (NISO+12)*MULT+1+NISO
CW
      +NGROUP*(2+ICHIST*(2/(ICHIST+1)))=NUMBER OF WORDS
С
CB
     FORMAT(4H 2D ,1H*,11A6,1H*
                                       HSETID, HISONM
CB
     11H*,A6,1H*,9(1X,A6)/(10(1X,A6))
CB
                                       CHI (PRESENT IF ICHIST.EQ.1)
     FORMAT(6E12.5)
CB
     FORMAT(6E12.5)
                                       VEL, EMAX, EMIN
CB
                                      LOCA
     FORMAT(12I6)
С
```

```
CD
     HSETID(I)
                 HOLLERITH IDENTIFICATION OF FILE (A6)
CD
     HISONM(I) HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6)
                 FILE-WIDE FISSION SPECTRUM(PRESENT IF ICHIST.EQ.1)
CD
     CHI(J)
CD
     VEL(J)
                 MEAN NEUTRON VELOCITY IN GROUP J (CM/SEC)
     EMAX(J)
CD
                 MAXIMUM ENERGY BOUND OF GROUP J (EV)
     EMIN
LOCA(I)
                MINIMUM ENERGY BOUND OF SET (EV)
CD
                NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR
CD
CD
                    ISOTOPE I.
C
C----
           FILE-WIDE CHI DATA (3D RECORD)
CR
C
CC
       PRESENT IF ICHIST.GT.1
C
CL
     ((CHI(K,J),K=1,ICHIST),J=1,NGROUP),(ISSPEC(I),I=1,NGROUP)
С
CW
     NGROUP*(ICHIST+1)=NUMBER OF WORDS
С
CB
     FORMAT(4H 3D ,1P5E12.5/(6E12.5)) CHI
CB
     FORMAT(12I6)
                                     ISSPEC
С
CD
     CHI(K,J) FRACTION OF NEUTRONS EMITTED INTO GROUP J AS A
CD
                    RESULT OF FISSION IN ANY GROUP, USING SPECTRUM K -
CD
     TO CALCULATE EMISSION SPECTRUM FROM FISSION
CD
CD
                    IN GROUP I
C
С
            ISOTOPE CONTROL AND GROUP INDEPENDENT DATA (4D RECORD)
CR
С
     HABSID, HIDENT, HMAT, AMSS, EFISS, ECAPT, TEMP, SIGPOT, ADENS, KBR, ICHI, -
CL
CL
    1IFIS, IALF, INP, IN2N, IND, INT, LTOT, LTRN, ISTRPD,
CL
    2(IDSCT(N), N=1, NSCMAX), (LORD(N), N=1, NSCMAX),
CL
    3((JBAND(J,N),J=1,NGROUP),N=1,NSCMAX),
CL
    4((IJJ(J,N),J=1,NGROUP),N=1,NSCMAX)
C
CW
     3*MULT+17+NSCMAX*(2*NGROUP+2)=NUMBER OF GROUPS
С
CB
     FORMAT(4H 4D ,3(1X,A6)/6E15.5/(12I6))
С
                 HOLLERITH ABSOLUTE ISOTOPE LABEL - SAME FOR ALL
CD
     HABSID
CD
                    VERSIONS OF THE SAME ISOTOPE IN FILE (A6)
CD
     HIDENT
                 IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA
CD
                   CAME (E.G. ENDF/B) (A6)
CD
     AMASS
                 GRAM ATOMIC WEIGHT
     EFISS
^{\rm CD}
                 TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)
CD
     ECAPT
                 TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/FISS)
```

CD	TEMP	ISOTOPE TEMPERATURE (DEGREES KELVIN)	_
CD	SIGPOT		_
CD		RESONANCE RANGE (BARNS/ATOM)	-
CD	ADENS	DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE	_
CD		CROSS SECTIONS WERE GENERATED (Δ/BARN-CM)	-
CD	KBR	ISOTOPE CLASSIFICATION	_
CD		O=UNDEFINED	_
CD CD		1=FISSILE 2=FERTILE	_
CD		2=FERILE 3=OTHER ACTINIDE	_
CD		4=FISSION PRODUCT	_
CD		5=STRUCTURE	_
CD		6=COOLANT	_
CD		7=CONTROL	_
CD	ICHI	ISOTOPE FISSION SPECTRUM FLAG	_
CD	10111	ICHI.EQ.O USE FILE-WIDE CHI	_
CD		ICHI.EQ.1 ISOTOPE CHI VECTOR	_
CD		ICHI.GT.1 ISOTOPE CHI MATRIX	_
CD	IFIS	(N,F) CROSS SECTION FLAG	_
CD	11 10	IFIS.EQ.O NO FISSION DATA IN PRINCIPAL	_
CD		CROSS SECTION RECORD	_
CD		IFIS.EQ.1 FISSION DATA PRESENT IN PRINCIPAL	_
CD		CROSS SECTION RECORD	_
CD	IALF	(N,ALPHA) CROSS SECTION	_
CD		SAME OPTIONS AS IFIS	_
CD	INP	(N,P) CROSS SECTION	_
CD		SAME OPTIONS AS IFIS	_
CD	IN2N	(N,2N) CROSS SECTION	_
CD		SAME OPTIONS AS IFIS	_
CD	IND	(N,D) CROSS SECTION	_
CD		SAME OPTIONS AS IFIS	_
CD	INT	(N,T) CROSS SECTION	_
CD		SAME OPTIONS AS IFIS	_
CD	LTOT	NUMBER OF MOMENTS OF TOTAL CROSS SECTION PROVIDED	-
CD		IN PRINCIPAL CROSS SECTIONS RECORD	_
CD	ITRN	NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION	_
CD		PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD	_
CD	ISTRPD	NUMBER OF COORDINATE DIRECTIONS FOR WHICH	_
CD		COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS	_
CD		ARE GIVEN. IF ISTRPD=0, NO COORDINATE DEPENDENT	_
CD		TRANSPORT CROSS SECTIONS ARE GIVEN.	_
CD	${\tt IDSCT(N)}$		-
CD		SCATTERING BLOCK N. SIGNIFICANT ONLY IF	-
CD		LORD(N).GT.O	-
CD		IDSCT(N)=000 + NN, TOTAL SCATTERING, (SUM OF	-
CD		ELASTIC, INELASTIC, AND N2N SCATTERING	-
CD		MATRIX TERMS).	-
CD		100 + NN, ELASTIC SCATTERING	-
CD		200 + NN, INELASTIC SCATTERING	-
CD		300 + NN, (N,2N) SCATTERING,SEE	-
CD		NOTE BELOW	_
CD		WHERE NN IS THE LEGENDRE EXPANSION INDEX OF THE	_
CD		FIRST MATRIX IN BLOCK N	-

```
CD
     LORD(N)
                  NUMBER OF SCATTERING ORDERS IN BLOCK N. IF
CD
                     LORD(N)=0, THIS BLOCK IS NOT PRESENT FOR THIS
CD
                     ISOTOPE. IF NN IS THE VALUE TAKEN FROM
CD
                     IDSCT(N), THEN THE MATICES IN THIS BLOCK
CD
                     HAVE LEGENDRE EXPANSION INDICES OF NN, NN+1,
CD
                     NN+2,...,NN+LORD(N)-1
CD
      JBAND(J.N) NUMBER OF GROUPS THAT SCATTER INTO GROUP J.
CD
                     INCLUDING SELF-SCATTER, IN SCATTERING BLOCK N.
CD
                     IF JBAND(J,N)=0, NO SCATTERING DATA IS PRESENT
CD
                     IN BLOCK N.
CD
      IJJ(J,N)
                  POSITION OF IN-GROUP SCATTERING CROSS SECTION IN
                     SCATTERING DATA FOR GROUP J, SCATTERING BLOCK
CD
                     N, COUNTED FROM THE FRIST WORD OF GROUP J DATA.
CD
CD
                     IF JBAND(J,N).NE.O THEN IJJ(J,N) MUST SATISFY
CD
                     THE RELATION 1.LE.IJJ(J,N).LE.JAND(J,N)
С
CD
                  NOTE- FOR N, 2N SCATTER, THE MATRIX CONTAINS TERMS,
CD
                     SCAT(J TO G), WHICH ARE EMISSION (PRODUCTION)-
CD
                     BASED, I.E., ARE DEFINED SUCH THAT MACROSCOPIC
                     SCAT(J TO G) TIMES THE FLUX IN GROUP J GIVES
CD
CD
                     THE RATE OF EMISSION (PRODUCTION) OF NEUTRONS
CD
                     INTO GROUP G.
C
C
C
            PRINCIPAL CROSS SECTIONS (5D RECORD)
CR
С
CL
      ((STRPL(J,L),J=1,NGROUP),L=1,LTRN),
     1((STOPL(J,L),J=1,NGROUP)L=1,LTOT),(SNGAM(J),J=1,NGROUP),
CL
CL
     2(SFIS(J), J=1, NGROUP), (SNUTOT(J), J=1, NGROUP),
CL
     3(CHISO(J), J=1, NGROUP), (SNALF(J), J=1, NGROUP),
CL
     4(SNP(J), J=1, NGROUP), (SN2N(J), J=1, NGROUP),
     5(SND(J), J=1, NGROUP), (SNT(J), J=1, NGROUP),
CL
CL
     6(STRPD(J,I),J=1,NGROUP),I=1,ISTRPD)
С
CW
      (1+LTRN+LTOT+IALF+INP+IN2N+IND+INT+ISTRPD+2*IFIS+
CW
      ICHI*(2/(ICHI+1)))*NGROUP=NUMBER OF WORDS
С
     FORMAT(4H 5D ,5E12.5/(6E12.5))
CB
C
CD
      STRPL(J,L) PL WEIGHTED TRANSPORT CROSS SECTION
CD
                     THE FIRST ELEMENT OF ARRAY STRPL IS THE
CD
                     CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION
CD
                     THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1)
                     IS NOT INCLUDED IN STRPL(J.L).
CD
CD
      STOTPL(J,L) PL WEIGHTED TOTAL CROSS SECTION
CD
                     THE FIRST ELEMENT OF ARRAY STOTPL IS THE
CD
                     FLUX (PO) WEIGHTED TOTAL CROSS SECTION
CD
                     THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1)
CD
                     IS NOT INCLUDED IN STRPL(J,L).
CD
      SNGAM(J)
                (N,GAMMA)
```

```
CD
                (N,F) (PRESENT IF IFIS.GT.0)
     SFIS(J)
                TOTAL NEUTRON YIELD/FISSION (PRESENT IF IFIS.GT.O)
CD
     SNUTOT(J)
CD
     SCHISO(J)
                ISOTOPE CHI (PRESENT IF ICHI.EQ.1)
CD
     SNALF(J)
                (N,ALPHA)
                             (PRESENT IF IALF.GT.0)
CD
     SNP(J)
                (N,P)
                             (PRESENT IF INP.GT.0)
CD
     SN2N(J)
                (N,2N)
                             (PRESENT IF IN2N.GT.0) ----SEE
CD
                                        NOTE BELOW----
     SND(J) (N,D)
SNT(J) (N,T)
CD
                             (PRESENT IF IND.GT.0)
CD
                             (PRESENT IF INT.GT.0)
CD
     STRPD(J,I) COORDINATE DIRECTION I TRANSPORT CROSS SECTION
CD
                             (PRESENT IF ISTRPD.GT.O)
С
                NOTE - THE PRINCIPAL N,2N CROSS SECTION SN2N(J)
CN
CN
                   IS DEFINED AS THE N,2N REACTION CROSS SECTION,
CN
                   I.E., SUCH THAT MACROSCOPIC 2N2N(J) TIMES THE
CN
                   FLUX IN GROUP J GIVES THE RATE AT WHICH N, 2N
CN
                   REACTIONS OCCUR IN GROUPJ. THUS, FOR N,2N
CN
                   SCATTERING, SN2N(J) = 0.5*(SUM OF SCAT(J TO G)
CN
                   SUMMED OVER ALL G).
С
C
          ISOTOPE CHI DATA (6D RECORD)
CR
C
CC
           PRESENT IF ICHI.GT.1
С
CL
     ((CHIISO(K,J),K=1,ICHI),J=1,NGROUP),(ISOPEC(I),I=1,NGROUP)
С
CW
     NGROUP*(ICHI+1)=NUMBER OF WORDS
C
     FORMAT(4H 6D ,5E12.5/(6E12.5)) CHIISO
CB
CB
     FORMAT(12I6)
                                   ISOPEC
С
CD
     CHIISO(K, J) FRACTION OF NEUTRONS EMITTED INTO GROUP J AS A
CD
                   RESULT OF FISSION IN ANY GROUP, USING SPECTRUM K
CD
     CD
                   TO CALCULATE EMISSION SPECTRUM FROM FISSION
CD
                   IN GROUP I
С
C-
С
           SCATTERING SUB-BLOCK (7D RECORD)
CR
С
CL
     ((SCAT(K,L),K=1,KMAX),L+1,LORDN
C
CC
     KMAX=SUM OVER J OF JBAND(J,N) WITHIN THE J-GROUP RANGE OF THIS
CC
        SUB-BLOCK. IF M IS THE INDEX OF THE SUB-BLOCK, THE J-GROUP
CC
        RANGE CONTAINED WITHIN THIS SUB-BLOCK IS
CC
        JL=(M-1)*((NGROUP-1)/NSBLOK+1)+1 TO JU=MINO(NGROUP, JUP),
```

```
CC
        WHERE JUP=M*((NGROUP-1)/NSBLOK+1).
С
CC
     LORDN=LORD(N)
     N IS THE INDEX FOR THE LOOP OVER NSCMAX (SEE FILE STRUCTURE)
CC
С
CW
     KMAX*LORDN=NUMBER OF GROUPS
С
CB
     FORMAT(4H 7D ,5E12.5/(6E12.5))
С
CD
     SCAT(K,L) SCATTERING MATRIX OF SCATTERING ORDER L, FOR
CD
                    REACTION TYPE IDENTIFIED BY IDSCT(N) FOR THIS
CD
                    BLOCK. JBAND(J,N) VALUES FOR SCATTERING INTO
CD
                    GROUP K ARE STORED AT ; PCATOPMS L=SUM FROM 1
                    TO (J-1)( OF JBAND(J,N) PLUS 1 TO K-1+JBAND(J,N). -
CD
CD
                    THE SUM IS ZERO WHEN J=1. J-TO-J SCATTER IS
CD
                    THE IJJ(J,N)-TH ENTRY IN THE RANGE JBAND(J,N).
CD
                    VALUES ARE STORED IN THE ORDER (J+JUP),
CD
                    (J+JUP-1),...,(J+1),J,(J-1),...,(J-JDN),
CD
                    WHERE JUP=IJJ(J,N)-1 AND JDN=JBAND(J,N)-IJJ(J,N). -
С
```

## Appendix G. GOXS FILE DESCRIPTION

The following description of the GOXS format uses the standard CCCC form. The GOXS format is the same as the MACRXS and SNXEDT formats used in the ONEDANT and TWODANT codes.

C***	******	*********	*********	***				
С		DATE 05/12/83		_				
С				_				
CF	GOX	S		_				
CE	GROUP-ORDERED CROSS SECTIONS FOR SN							
C				_				
CN		THIS FILE CONTAINS	CROSS SECTION	_				
CN	THIS FILE CONTAINS CROSS SECTION TRANSPORT TABLES AND RESPONSE EDITS							
CN		IN A GROUP-ORDERED		_				
CN		FOR USE IN SN TRANS		_				
C		TON ODD IN DA IMME	TOTAL CODED.	_				
•	****	*********	*********	k**				
C	1-1-1-1-1-1-1-1-1-1-1-1-1-1							
C								
C								
CS	ם זדים	STRUCTURE		_				
CS	1 111	SIROGIGIE		_				
CS		RECORD TYPE	PRESENT IF	_				
CS				_				
CS		FILE IDENTIFICATION	ALWAYS	_				
CS		FILE CONTROL	ALWAYS	_				
CS		FILE CONTROL FILE DATA	ALWAYS					
		***(REPEAT FOR ALL GROUPS)	ALWAIS					
CS		EDIT CROSS SECTIONS	AT LIAVO	_				
			ALWAYS					
CS		SCATTERING CONTROL	NORD.GT.O	_				
CS	* SCATTERING DATA NORD.GT.O  ***********************************							
	******	*****		_				
C				_				
C								
C								
C								
C								
CR	FIL	E IDENTIFICATION		_				
C	/			_				
	HNAME, (HUS	E(I),I=1,2),IVERS		_				
С				_				
CW	1+3*MULT			-				
С	_			-				
CB	FORMAT(4H	OV ,A8,1H*,2A8,1H*,I6)		-				
С				-				
CD	HNAME	HOLLERITH FILE NAME - G	` '	-				
CD	HUSE	HOLLERITH USER IDENTIFIA	TION (8A)	-				
CD	IVERS	FILE VERSION NUMBER		-				
CD	MULT	DOUBLE PRECISION PARAMET	'ER	-				
CD		1- A8 WORD IS SINGL	E WORD	-				
CD		2- A8 WORD IS DOUBL	E PRECISION WORD	-				

```
С
С
C
              FILE CONTROL
CR
С
CL
       NGROUP, NMAT, NORD, NED, IDPF, LNG, MAXUP, MAXDN, NPRIN, I2LP1
C
CW
       10
C
CD
       NGROUP
                      NUMBER OF GROUPS
       NMAT
                      NUMBER OF MATERIALS
CD
       NORD NUMBER OF LEGENDRE ORDERS
NED NUMBER OF EXTRA EDIT CROSS SECTIONS
CD
CD
CD
                      (IN ADDITION TO THE BASIC PRINCIPAL CROSS SECTIONS)
      IDPF DOUBLE PRECISION FLAG FOR EDIT AND SCATTERING DATA
CD
CD
                          (1/2=SINGLE/DOUBLE)
CD LNG
                    LAST NEUTRON GROUP FOR COUPLED SETS
   MAXUP MAXIMUM NUMBER OF UPSCATTER GROUPS
MAXDN MAXIMUM NUMBER OF DOWNSCATTER GROUPS
NPRIN NUMBER OF PRINCIPAL CROSS SECTIONS (0, 4, OR 5)
12LP1 2L+1 TERM INCLUDED IN LIBRARY (0/1=NO/YES)
^{\rm CD}
CD
CD
CD
C
           FILE DATA
С
     (HMAT(I), I=1,NMAT), (HED(J), J=1, NEDT), (VEL(K), K=1, NGROUP),
CL
CL
      1(EG(K), K=1, NGROUP), EMIN
С
CW
    (NMAT+NED)*MULT+2*NGROUP+1
С
   HMAT(I) HOLLERITH MATERIAL NAMES
HED(J) HOLLERITH EDIT CROSS SECTION NAMES
VEL(K) AVERAGE VELOCITY FOR GROUP K (CM/SEC)
EG(K) MAX ENERGY BOUND FOR GROUP K (EV)
EMIN MIN ENERGY BOUND FOR GROUP STRUCTURE (EV)
CD
^{\rm CD}
CD
CD
CD EMIN
CD NEDT
                    NED+NPRIN
C
С
      EDIT CROSS SECTIONS
CR
С
CL ((EDXS(I,J),I=1,NMAT),J=1,NEDT)
C
CW
       NMAT*NEDT
С
       EDXS(I,J) EDIT CROSS SECTIONS. THE FOLLOWING 4 REACTIONS
CD
```

```
CD
                ARE ALWAYS PRESENT IN THIS ORDER WHEN NPRIN=4:
CD
                   TOTAL TOTAL TRANSPORT XSEC
CD
                   ABS
                            BALANCE ABSORPTION XSEC
CD
                   NUSIGF FISSION NEUTRON PRODUCTION XSEC
CD
                   CHI
                           FISSION SPECTRUM
CD
                ALSO PRESENT WHEN NPRIN=5:
CD
                           TRANSPORT FOR DIFFUSION
CD
                ANY EXTRA EDITS FOLLOW THESE STANDARD EDITS.
CD
                WHEN NPRIN=O, ANY NAMES ARE ALLOWED.
С
С
C
CR
     SCATTERING CONTROL
С
CL ((NJJ(L,I),L=1,NORD),I=1,NMAT),
CL 1((IJJ(L,I),L=1,NORD),I=1,NMAT)
С
CW
   2*NORD*NMAT
С
CD NJJ(L,I) NUMBER OF GROUPS IN BAND
CD IJJ(L,I) FIRST GROUP IN BAND
С
С
         SCATTERING DATA
С
CL SCAT(I), I=1,NTAB)
C
CW NTAB
С
CD SCAT(K) SCATTERING DATA.
CD NTAB SUM OF NJJ(L,I) OVER L FROM 1 TO NORD AND
CD
                 I FROM 1 TO NMAT
С
```

## Appendix H. EXAMPLE OF A MATXS INDEX FILE

The following text is part of the index for MATXS10, the 30 x 12 library based on ENDF/B-VI. Sections that were removed are marked with ellipses.

*******	******	*********
*** FILE	MATXS	******
*** USER	T2LANL NJOY	*********
*** VERS	10	*********
*******	******	******

## FILE DESCRIPTION

30X12 LIBRARY FROM ENDF/B-VI, JAN 1992 P4, 300K AT INFINITE DILUTION STANDARD CLAW WEIGHT FUNCTION

## FILE DATA

PARTICLE	NAME	NGRP	
1	 N	30	
2	G	12	
DATA TYPE	NAME	JINP	JOUTP
1	NSCAT	1	1
2	NG	1	2
3	GSCAT	2	2
MATERIAL	HMAT	NSUB	LOCA
1	H1	3	0
2	H2	3	16
3	Н3	2	34
4	HE3	2	49
5	HE4	2	62
6	LI6	3	75
7	LI7	3	153
8	BE9	3	231
9	B10	3	250
10	B11	3	330
11	CNAT	3	388
12	N14	3	426
13	N15	3	511
14	016	3	562
15	017	2	644
16	F19	3	689
17	NA23	3	760
18	MGNAT	3	820

19	MG24	2	926
20	AL27	3	937
21	SINAT	3	1033
22	SI28	3	1110
23	P31	3	1267
		3	1290
24	SNAT		
25	S32	3	1395
26	CLNAT	3	1418
27	AR4O	2	1494
28	KNAT	3	1505
29	K41	2	1603
30	CANAT	3	1614
31	SC45	2	1686
32	TINAT	3	1697
33	TI46	2	1746
34	TI47	2	1757
35	TI48	2	1768
36	VNAT	3	1779
37	CR50	3	1852
38	CR52	3	1912
39	CR53	3	1987
40	CR54	3	2075
41	MN55	3	2119
<b>4</b> 2	FE54	3	2271
<b>4</b> 3	FE58	3	2334
44	C059	3	2377
<b>4</b> 5	NI58	3	2440
<del>4</del> 6	NI59	2	2507
47	NI60	3	2518
<b>4</b> 8	NI61	3	2598
<b>4</b> 9	NI62	3	2661
50	NI64	3	2712
51	CU63	3	2755
52	CU65	3	2878
53	GANAT	3	2965
54	Y89	3	2986
55	NB93	3	3035
56	MONAT	3	3112
57	CDNAT	3	3135
58	INNAT	3	3172
59	BA138	3	3259
60	EU151	3	3282
61	EU153	3	3343
62	EU155	2	3390
63	HO165	3	3431
			3484
64	HFNAT	2	
65	TA181	3	3525
66	W182	3	3568
67	W183	3	3636
68	W184	3	3694
69	W186	3	3760
70	W100 RE185		
		2	3826
71	RE187	2	3863

72	AU197	3	3914
73	PB206	3	3967
74	PB207	3	4150
75	PB208	3	4333
76	BI209	3	4404
77	TH230	2	4473
78	TH232	3	4529
79		2	
	PA231		4588
80	PA233	2	4634
81	U232	2	4682
82	U233	3	4730
83	U234	2	4770
84	U235	3	4808
85	U236	2	4908
86	U238	3	4988
87	NP237	3	5075
88	NP238	2	5225
89	NP239	2	5238
90	PU236	2	5270
91	PU237	2	5302
92	PU238	2	5346
93	PU239	3	5400
93 94	PU239 PU240	3	5494
9 <del>1</del> 95			
	PU241	3	5564
96	PU242	3	5623
97	PU243	3	5690
98	PU244	2	5718
99	AM241	3	5752
100	AM242	2	5816
101	AM242M	3	5831
102	AM243	3	5888
103	CM241	2	5953
104	CM242	3	5983
105	CM243	3	6020
106	CM244	3	6081
107	CM245	3	6118
108	CM246	3	6144
109	CM247		6192
110	CM248	3 3	6218
	BK249	2	6263
111			
112	CF249	2	6315
113	CF250	3	6367
114	CF251	3	6393
115	CF252	3	6419
116	CF253	2	6445
117	ES253	2	6458

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H1 SUB 1 3.000E+02 1.000E+10 NSCAT

VECTORS: NWTO NTOTO NELAS NG HEAT KERMA DAME MUBAR

XI GAMMA INVEL

MATRICES: NELAS

H1 SUB 2 3.000E+02 1.000E+10 NG

MATRICES: NG

H1 SUB 3 0.000E+00 1.000E+10 GSCAT

VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT

MATRICES: GCOH GINCH GPAIR

\_\_\_\_\_

H2 SUB 1 3.000E+02 1.000E+10 NSCAT

VECTORS: NWTO NTOTO NELAS N2N NG HEAT KERMA DAME

MUBAR XI GAMMA INVEL

MATRICES: NELAS N2N

H2 SUB 2 3.000E+02 1.000E+10 NG

MATRICES: NG

H2 SUB 3 0.000E+00 1.000E+10 GSCAT

VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT

MATRICES: GCOH GINCH GPAIR

\_\_\_\_\_

H3 SUB 1 3.000E+02 1.000E+10 NSCAT

VECTORS: NWTO NTOTO NELAS N2N HEAT KERMA DAME MUBAR

XI GAMMA INVEL

MATRICES: NELAS N2N

H3 SUB 2 0.000E+00 1.000E+10 GSCAT

VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT

MATRICES: GCOH GINCH GPAIR

\_\_\_\_\_

HE3 SUB 1 3.000E+02 1.000E+10 NSCAT

VECTORS: NWTO NTOTO NELAS NG NP ND HEAT KERMA

DAME MUBAR XI GAMMA INVEL

MATRICES: NELAS

HE3 SUB 2 0.000E+00 1.000E+10 GSCAT

VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT

MATRICES: GCOH GINCH GPAIR

HE4 SUB 1 3.000E+02 1.000E+10 NSCAT

VECTORS: NWTO NTOTO NELAS HEAT KERMA DAME MUBAR XI

GAMMA INVEL

MATRICES: NELAS

SUB 2 0.000E+00 1.000E+10 GSCAT HE4 VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT MATRICES: GCOH GINCH GPAIR LI6 SUB 1 3.000E+02 1.000E+10 NSCAT VECTORS: NWTO NTOTO NELAS NINEL N2NA NO1D NO2D NO3D NO4D NO5D NO6D NO7 NO8D NO9D N10D N11D N12D N13D N14D N15D N16D N17D N18D N19D 
 N20D
 N21D
 N22D
 N23D
 N24D
 N25D
 N26D
 N27D

 N28D
 N29D
 NG
 NP
 NT
 HEAT
 KERMA
 DAME
 MUBAR XI GAMMA INVEL MATRICES: NELAS N2NA N01D N02D N03D N04D N05D N06D NO8D NO9D N10D N11D N12D N13D N14D NO7 N15D N16D N17D N18D N19D N20D N21D N22D N23D N24D N25D N26D N27D N28D N29D LI6 SUB 2 3.000E+02 1.000E+10 NG MATRICES: NO7 NG SUB 3 0.000E+00 1.000E+10 GSCAT VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT MATRICES: GCOH GINCH GPAIR LI7 SUB 1 3.000E+02 1.000E+10 NSCAT VECTORS: NWTO NTOTO NELAS NINEL N2N N2NA N3NA N01 
 NO2T
 NO3T
 NO4T
 NO5T
 NO6T
 NO7T
 NO8T
 NO9T

 N10T
 N11T
 N12T
 N13T
 N14T
 N15T
 N16T
 N17T
 N18T N19T N20T N21T N22T N23T N24T N25T ND HEAT KERMA DAME MUBAR N26T N27T NG GAMMA INVEL XI MATRICES: NELAS N2N N2NA N3NA N01 N02T NO3T NO4T NO5T NO6T NO7T NO8T NO9T N10T N11T N12T N13T N14T N15T N16T N17T N18T N19T N20T N21T N22T N23T N24T N25T N26T N27T SUB 2 3.000E+02 1.000E+10 NG LI7 MATRICES: NO1 NG SUB 3 0.000E+00 1.000E+10 GSCAT LI7 VECTORS: GWTO GTOTO GCOH GINCH GPAIR GABS GHEAT MATRICES: GCOH GINCH GPAIR

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	VECTORS: MATRICES:	NWTO NA MT800 NELAS	3.000E+02 NTOTO HEAT MUBAR N2N 3.000E+02	NELAS KERMA XI	N2N DAME GAMMA	NG MT600 INVEL	NP		NT PO1
БЦе	MATRICES:			1.	0001.10	14 G			
BE9	VECTORS:	GWTO	O.000E+00 GTOTO GINCH	GCOH				GHEAT	
B10		NWTO NO5A N13A N21DAA N29DAA DAME MT8O1 NELAS NO8A N16A	MUBAR NO1	NELAS NO7 N15P N23DAA NP MT601 XI NO2 N10A		NO1 NO9A N17A N25A NA MT6O3 INVEL NO4 N12DAA N2ODAA	NO2 N10A N18DAA N26DAA NT2A MT604	N11A N19A N27DAA HEAT MT605 N06A N14DAA	NO4 N12DAA N20DAA N28P KERMA MT800 N07 N15P N23DAA
B10			3.000E+02 MT801			NG			
B10	VECTORS:	GWTO	O.000E+00 GTOTO GINCH	GCOH				GHEAT	
• • •									
U235	SUB : VECTORS:	NWTO NNF NO6 N14 N22 N30	3.000E+02 NTOTO N2NF N07 N15 N23 N31	NELAS N3NF N08 N16 N24 N32	000E+10 NINEL N01 N09 N17 N25	NSCAT N2N NO2 N10 N18 N26 N34	N3N N03 N11 N19 N27 NCN	NFTOT NO4 N12 N20 N28 NG	NF NO5 N13 N21 N29 HEAT
	MATRICES:	KERMA NELAS NO7		XI NO1 NO9	GAMMA NO2 N10	INVEL NO3 N11	NUDEL NO4 N12	CHID NO5 N13	NO6 N14

		N15 N23 N31	N16 N24 N32	N17 N25 N33	N18 N26 N34	N19 N27 N2N	N20 N28 N3N	N21 N29 NCN	N22 N30
U235	SUB MATRICES	2 : NINEL	3.000E+02 NFTOT	NG	1.000E+10 NNONEL	NG			
U235	SUB VECTORS: MATRICES	3 GWTO : GCOH	0.000E+00 GTOTO GINCH	GCOH GPAII	1.000E+10 GINCH R	GSCAT GPAIR	GABS	GHEAT	

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INDEX COMPLETE 2555.6S

A complete listing of this file is included in the TRANSX 2.0 distribution package.