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SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation

Functional Modules
F1 - F8

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*Obsolete with SCALE-4.0 release.

PREFACE

Background

This Manual represents Revision 4 of the user documentation for the modular code system referred to as SCALE. The history of the SCALE code system dates back to 1969 when the current Computing Applications Division at Oak Ridge National Laboratory (ORNL) began providing the transportation package certification staff at the U.S. Atomic Energy Commission with computational support in the use of the new KENO code for performing criticality safety assessments with the statistical Monte Carlo method. From 1969 to 1976 the certification staff relied on the ORNL staff to assist them in the correct use of codes and data for criticality, shielding, and heat transfer analyses of transportation packages. However, the certification staff learned that, with only occasional use of the codes, it was difficult to become proficient in performing the calculations often needed for an independent safety review. Thus, shortly after the move of the certification staff to the U.S. Nuclear Regulatory Commission (NRC), the NRC staff proposed the development of an easy-to-use analysis system that provided the technical capabilities of the individual modules with which they were familiar. With this proposal, the concept of the Standardized Computer Analyses for Licensing Evaluation (SCALE) code system was born.

The NRC staff provided ORNL with some general development criteria for SCALE: (1) focus on applications related to nuclear fuel facilities and package designs, (2) use well-established computer codes and data libraries, (3) design an input format for the occasional or novice user, (4) prepare "standard" analysis sequences (control modules) that will automate the use of multiple codes (functional modules) and data to perform a system analysis, and (5) provide complete documentation and public availability. With these criteria the ORNL staff laid out the framework for the SCALE system and began development efforts. The initial version (Version 0) of the SCALE Manual was published in July 1980. Then, as now, the Manual is divided into three volumes – Volume 1 for the control module documentation (Sections C4, S1– S4, and H1), Volume 2 for the functional module documentation (Sections F1– F16), and Volume 3 for the documentation of the data libraries and subroutine libraries (Sections M1–M16).

System Overview

The original concept of SCALE was to provide "standardized" sequences where the user had very few analysis options in addition to the geometry model and materials. Input for the control modules has been designed to be free-form with extensive use of keywords and engineering-type input requirements. The more flexible functional modules have a more difficult input logic and require the user to interface the data sets necessary to run the modules in a stand-alone fashion. As the system has grown in popularity over the years and additional options have been requested, the control modules have been improved to allow sophisticated users additional access to the numerous capabilities within the functional modules. However, the most important feature of the SCALE system remains the capability to simplify the user knowledge and effort required to prepare material mixtures and to perform adequate problem-dependent cross-section processing.

The modules available in Version 0 of SCALE were for criticality safety analysis sequences (CSAS) that provided automated material and cross-section processing prior to a one-dimensional (1-D) or multidimensional criticality analysis. Since that time the capabilities of the system have been significantly expanded to provide additional CSAS capabilities, new shielding analysis sequences (SAS) that also include depletion/decay capabilities for spent fuel characterization, and a heat transfer analysis sequence (HTAS). At the center of the CSAS and SAS sequences is the library of subroutines referred to as the Material Information Processor or MIPLIB (see Section M7). The purpose of MIPLIB is to allow users to specify problem materials using easily remembered and easily recognizable keywords that are associated with mixtures, elements, and nuclides provided in the Standard Composition Library (see Section M8). MIPLIB also uses other keywords

and simple geometry input specifications to prepare input for the modules that perform the problem-dependent cross-section processing: BONAMI, NITAWL-II, and XSDRNPM. A keyword supplied by the user selects the cross-section library from a standard set provided in SCALE (see Section M4) or designates the reference to a user-supplied library. Several utility modules from AMPX[1] have been added to this version of SCALE to provide users with the capability to edit the cross-section data and reformat user-supplied libraries for use in SCALE.

Over the history of the project several modules have been removed from the system because they are no longer supported by the development staff at ORNL. Tables 1 and 2 provide a summary of the major applications of each of the control modules and functional modules currently in the SCALE code system. The control modules were designed to provide the system analysis capability originally requested by the NRC staff. The CSAS module (sometimes denoted as the CSAS4 module and documented in Section C4) is currently the only control module designed for the calculation of the neutron multiplication factor of a system. Eight sequences enable general analysis of a 1-D system model or a multidimensional system model, capabilities to search on geometry spacing, and problem-dependent cross-section processing for use in executing stand-alone functional modules. The SAS1 and SAS3 modules (see Sections S1 and S3, respectively) provide general 1-D deterministic and 3-D Monte Carlo analysis capabilities. The SAS2 module (see Section S2) was originally developed to perform a depletion/decay calculation to obtain spent fuel radiation source terms that were subsequently input automatically to a 1-D, radial shielding analysis in a cylindrical geometry. Over time the depletion/decay portion of the SAS2 module has been significantly enhanced and interfacing to the other shielding modules has been provided. The SAS4 module (see Section S4) enables automated particle biasing for a Monte Carlo analysis of a transportation package-type geometry. The HTAS1 module (see Section H1) is the only heat transfer control module and uses the various capabilities of the HEATING code to perform different sequences of steady-state and transient analysis that enable the normal and accident conditions of a transportation package to be evaluated. Like SAS4, the HTAS1 module is limited to a package-type geometry.

Portability

Version 4.2 of the SCALE system has been developed to ensure portability among various computing platforms. The system is maintained and enhanced at ORNL under quality assurance and configuration management plans. The system has been routinely tested on IBM mainframe and IBM workstations. In addition, the system has been applied at ORNL on DEC and SUN workstations. Information needed to install SCALE on each of these systems is included with the software package distributed by the code centers. Advice for installation on HP workstations is also included in the software package. A separate SCALE software package, designated SCALE-PC, is available for the execution of select portions of the SCALE system on a personal computer.

Related Developments

The definition of "easy-to-use" has changed considerably since the late 1970s. As funding has allowed, the ORNL development staff has sought to develop user interfaces that provide a distinct aid to novice or occasional users of the system. These full-screen input processors were developed to work on a personal computer and provide interactive help to the user in preparing accurate input for a SCALE module. Currently, input processors are available only for the criticality control sequences[2] and the ORIGEN-S functional module.[3]

The capability to perform a point-kernel shielding analysis within the SCALE system has been developed[4] and will be provided within SCALE-PC in the next release of the software package.

A 238-energy-group neutron cross-section library based on ENDF/B-V has recently been prepared for the SCALE system.[5] All the nuclides that are available in ENDF/B-V are in the library. A 44-group

library has been collapsed from this 238-group library and validated against numerous critical measurements.[6] These libraries are available as separate data packages from the software distribution centers.

Availability

The SCALE code system and the other software designated under Related Developments have been packaged by the Radiation Shielding Information Center (RSIC) under cooperative agreement with the Energy Science and Technology Software Center. The SCALE system and the related software may be obtained by contacting either

Energy Science and Technology Software Center
P.O. Box 1020
Oak Ridge, TN 37831-1020
Telephone: (615) 576-2606
FAX: (615) 576-2865

or

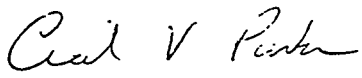
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Acknowledgments

The SCALE system is maintained at ORNL and enhanced to keep pace with normal technical advancements in the analysis areas of interest. Although the NRC continues its role as the controlling sponsor of the SCALE system, the U.S. Department of Energy (DOE) began assisting in the maintenance of the SCALE system in 1987. Over the years numerous individuals within these sponsoring organizations have played key roles in ensuring that the SCALE system remained a readily available, reliable system for the analysis of nuclear fuel facilities and packages. The individuals who have worked with the ORNL staff to coordinate maintenance and development activities include R. H. Odegaarden (NRC, ret.), G. H. Bidinger (NRC, ret.), C. Mauck (DOE, ret.), E. P. Easton (NRC), W. H. Lake (NRC and DOE), M. E. Wangler (DOE), and M. G. Bailey (NRC).

As demonstrated by this Manual, there are also numerous individuals from the ORNL staff who have contributed significantly to the development and enhancement of the SCALE system. Most are credited by their authorship of the sections in this Manual that correspond to their work. A few individuals have been essential to the development and maintenance of SCALE but are not credited by authorship. These individuals include: S. M. Bowman, who is responsible for proper configuration and testing of the development and production systems at ORNL and is the principal contact for general user assistance and training; S. K. Martin, who is responsible for implementing system changes; C. H. Shappert, who provided the editorial review of this Manual; and L. F. Norris, who prepared the entire manuscript. Special acknowledgement is also due to R. M. Westfall and G. E. Whitesides who, together with R. H. Odegaarden of the NRC, developed the concept and long-range goals of the SCALE system in the late 1970s. Finally, this Project Leader will always be grateful to L. M. Petrie, who for nearly 20 years has consistently provided consultation and advice on the technical

direction that should be taken in development of nearly every module and cross-section library that are in the present system.



Cecil V. Parks
SCALE Project Manager
March 1995

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Table 1 Analysis capabilities summary of the SCALE control modules

Control module	Analysis function(s)	Functional modules executed	Section reference
CSAS	1-D deterministic calculation of neutron multiplication 3-D Monte Carlo calculation of neutron multiplication Problem-dependent cross-section processing Multiplication search or spacing	BONAMI NITAWL-II XSDRNPM KENO V.a ICE	C4
SAS1	1-D deterministic calculation of radiation transport through shield and dose evaluation at a point Calculation of dose at detector based on leakage from critical volume	BONAMI NITAWL-II XSDRNPM XSDOSE	S1
SAS2	Point depletion/decay of nuclear fuel 1-D radial shielding analysis in cylindrical geometry	BONAMI NITAWL-II XSDRNPM COUPLE ORIGEN-S XSDOSE	S2
SAS3	Dose evaluation using MORSE Monte Carlo code	BONAMI NITAWL-II XSDRNPM MORSE-SGC	S3
SAS4	Calculation of dose outside of transportation package using MORSE code and automated biasing techniques	BONAMI NITAWL-II XSDRNPM MORSE-SGC	S4
HTAS1	R-Z steady-state and transient analyses of a transportation package	OCULAR HEATING	H1

Table 2 Analysis capabilities summary of the SCALE functional modules

Module	Function	Section reference
BONAMI	Resonance self-shielding of cross sections with Bondarenko factors	F1
NITAWL-II	Resonance self-shielding of cross sections with resolved resonance data	F2
XSDRNPM	General 1-D, discrete-ordinates code for: • zone-weighting of cross sections • eigenvalue calculations for neutron multiplication • fixed-source calculation for shielding analysis • adjoint calculation for determining importance functions	F3
XSDOSE	Module for calculation of dose at a point based on the 1-D leakage flux from a finite shield	F4
COUPLE	Interface module for preparation of cross-section and spectral data for ORIGEN-S	F6
ORIGEN-S	General-purpose point-depletion and decay code to calculate isotopic, decay heat, radiation source terms, and curie levels	F7
ICE	Cross-section utility module for mixing cross sections	F8
MORSE-SGC	Monte Carlo code with combinatorial and array geometry features used to perform radiation shielding analysis	F9
HEATING7.2	Finite-volume, multidimensional code for conduction and radiation heat transfer	F10
KENO V.a	Monte Carlo code for calculation of neutron multiplication factors	F11
OCULAR	Calculation of radiation exchange factors	F16

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Computing Applications Division

BONAMI: RESONANCE SELF-SHIELDING BY THE BONDARENKO METHOD

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ABSTRACT

BONAMI is a module of the SCALE system which is used to perform Bondarenko calculations for resonance self-shielding. Cross sections and Bondarenko factor data are input from an AMPX master library. The output is written as an AMPX master library. A wide variety of options is provided for different lattices and cell geometries through the use of Dancoff approximations. A novel interpolational scheme is used which avoids many of the problems of the widely employed Lagrangian schemes.

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F1.1 INTRODUCTION

BONAMI (BONdarenko AMPX Interpolator) is a module that accesses an AMPX[1] master data set that contains Bondarenko factors, performs a resonance self-shielding calculation based on the Bondarenko method, and produces problem-dependent master data sets. The capabilities and features in BONAMI roughly parallel the resonance self-shielding provisions in the SPHINX[2] and TDOWN[3] codes. This version of BONAMI is equivalent to versions released with the AMPX-77 code package.

BONAMI solves problems in a one-dimensional (1-D) multizone slab, cylindrical, or spherical geometry. In addition, the user can specify a one-or-more-zone homogeneous geometry, in which case the code makes one or more separate, independent, infinite medium calculations. A variety of "Dancoff expressions" (most of them borrowed from the SPHINX[2] code) are provided to take into account heterogeneous effects. For these expressions, zones can be designated as fuel, moderator, and, in some cases, cladding regions. BONAMI will use these designators to collect and process cross sections into the parameters required by the particular expression.

BONAMI requires an AMPX master library, which includes the Bondarenko data, for its cross-section data. Using this library and a description of the geometry of the system, the self-shielding calculation is made via an iterative process. Self-shielded cross-section values are placed into master library format and written on a new library, which also contains all data sets not used in the Bondarenko calculation but which are on the input master library. Nuclides that occur in more than one zone will have a unique data set created for every zone in which they occur.

The major advantages of the Bondarenko approach are its simplicity and speed. It is especially attractive for many fast reactor applications, which operate in an energy regime where the narrow resonance approximation is apt to be inadequate.

F1.2 THEORY

In multigroup resonance self-shielding calculations, one is interested in calculating effective cross sections of the form:

$$\overline{\sigma_g} = \frac{\int_g du\, \sigma(u)\, \phi(u)}{\int_g du\, \phi(u)} . \qquad \text{(F1.2.1)}$$

Since the cross section is generally known (from resonance parameters, tabular data, etc.), resonance self-shielding involves a determination of the flux, $\phi(u)$.

The basic equation on which the Bondarenko method[4] is based is a very simple expression for the flux in an infinite homogeneous medium:

$$\phi(u) = \sim \frac{1}{\Sigma_t(u)} \qquad \text{(F1.2.2)}$$

where $\phi(u)$ is the flux per unit lethargy u, and $\Sigma_t(u)$ is the macroscopic total cross section.

Equation (F1.2.2) can be obtained in several ways. The expression[5] for the collision density in an infinite medium having a small absorption cross section can be reduced through a series of assumptions to this form. A more direct method is to invoke the narrow resonance approximation which assumes that collision density is unaffected by a very narrow resonance and is, therefore, constant:

$$F(u) \equiv \Sigma_t(u)\ \phi(u) = \text{constant.}$$

For the Bondarenko approach, it is convenient to modify the form of the expression

$$\overline{\sigma_g^i} = \frac{\int_g du \frac{\sigma^i(u)}{\Sigma_t(u)}}{\int_g du \frac{1}{\Sigma_t(u)}}$$

to

$$\overline{\sigma_g^i} = \frac{\int_g du \frac{\sigma^i(u)}{N_i \sigma_t^i(u) + \sum_{j \neq i} N_j \sigma_t^j(u)}}{\int_g du \frac{1}{N_i \sigma_t^i(u) + \sum_{j \neq i} N_j \sigma_t(u)}}, \qquad \text{(F1.2.3)}$$

where i designates the nuclide of interest, N is the nuclide number density, and σ_t is the microscopic total cross section. If we divide the numerator and denominator of Eq. (F1.2.3) by N_i and define

$$\sigma_0^i \equiv \sum_{j \neq i} N_j \sigma_t^j(u)/N_i$$

the following expression is derived:

$$\overline{\sigma_g^i} = \frac{\int_g du \frac{\sigma^i(u)}{\sigma_t^i(u) + \sigma_0^i(u)}}{\int_g du \frac{1}{\sigma_t^i(u) + \sigma_0^i(u)}} . \qquad \text{(F1.2.4)}$$

The σ_0^i term is the cross section per atom of the nuclide i for all nuclides in the mixture other than nuclide i itself.

The cross sections for a specific process implied by Eq. (F1.2.4) are a function of three variables (other than the nuclide's own cross sections):

1. energy group,
2. temperature (Doppler broadening), and
3. σ_0.

The Bondarenko method ignores some fine structure by using an effective constant value for σ_0 within an energy group. This method allows one to precalculate cross sections without having to know the detailed composition in which they might be used.

The resonance shielding factors themselves are defined in straightforward fashion. First, define the infinite dilution average values for a process:

$$\overline{\sigma_g}\,\mathrm{ID} = \frac{\int_g du\, \sigma(u)}{\int_g du} .$$

This expression reduces from Eq. (F1.2.4) for $\sigma_0 = \infty$.

For a finite value of σ_0 and temperature T, the "Bondarenko factors" or "f-factors," $F_g(\sigma_0,T)$, are defined by

$$\overline{\sigma_g}(\sigma_0,T) \equiv F_g(\sigma_0,T)\,\overline{\sigma_g}\,\mathrm{ID} . \qquad \text{(F1.2.5)}$$

If one calculates cross sections at several values of σ_0 and temperature, it is possible to determine values for intermediate σ_0's and temperatures by interpolating in these tables. BONAMI uses a newly developed scheme for this interpolation, which is discussed in detail in Sect. F1.3 of this report.

In practice, factors are generated for important processes (generally fission, capture, elastic scattering, transport, and total) at five or six σ_0's, spanning the typical range encountered for the nuclide and at three or four temperatures. For a given temperature, the lower the values of σ_0 the more resonance shielding, and, hence, the lower the value of the f-factor.

F1.2.1 HETEROGENEOUS EFFECTS

Equation (F1.2.4) is used directly for the homogeneous case. For the heterogeneous case, the effects of leakage (or intrazone slowing down) can be included by the addition of an "effective escape cross section" to the σ_0 term. This heterogeneous treatment follows from the "second equivalence theorem of resonance escape," which states that a heterogeneous lattice characterized by an escape cross section σ_e has the same resonance integral as a homogeneous mixture with a background cross section of $\sigma_0 + \sigma_e$. For a convex body, the Wigner rational approximation for the escape cross section is

$$\sigma_e = \frac{1}{\bar{\ell} N_i}, \qquad \text{(F1.2.6)}$$

where $\bar{\ell}$ is the mean chord length in the body (equal to 4 Volume/Surface Area) and N_i is the number density of the nuclide being calculated.

In many reactors, fuel cells are arranged in a regular geometry of repeating cells. The presence of these cells in the neighborhood of other cells will, of course, affect the flux seen by an individual cell, resulting in additional self-shielding of the resonance cross sections. This effect is typically accounted for by using Dancoff factors. The Dancoff factor modifies $\bar{\ell}$ in the definition of σ_e. The σ_e is sometimes designated σ_H or Σ_H because it accounts for heterogeneous (H) effects.

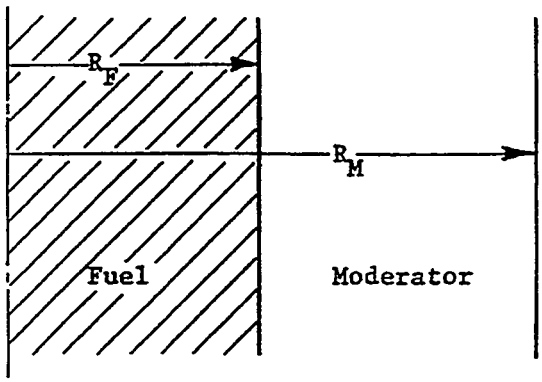
BONAMI has included several Dancoff expressions that account for different cell pin and cell lattice geometries.

The first eight options in BONAMI parallel those in the SPHINX[2] program, and are triggered by a parameter, ISSOPT:

1. Homogeneous Option (ISSOPT = 0 or 1000)

   In this option, an infinite homogeneous region is treated. (One can specify multiple zones in the BONAMI case and have each zone treated with an independent homogeneous calculation.)

2. Cylindrical Cell Using Sauer's Approximation[6] for the Dancoff Correction in a Hexagonal Lattice (ISSOPT = 1 or 1001)



In this case, the mean chord length ($\bar{\ell}$) in the lump is given by

$$\bar{\ell} = 2R_F .$$

The Dancoff factor is given by

$$C = \exp(-\tau\Sigma_M \bar{\ell}\, V_M/V_F)/(1 + (1-\tau)\Sigma_M \bar{\ell}\, V_M/V_F) ,$$

where V_M, V_F are the volumes of the moderator and fuel, respectively; Σ_M is the macroscopic total cross section in the moderator, and τ is a geometric index parameter which is given by

$$\tau = \left(\sqrt{\frac{\pi}{4\alpha}}\sqrt{1+V*} - 1\right)\frac{1}{V*} - \tau_0 ,$$

where $V* = \dfrac{V_M}{V_F}$ and α and τ_0 vary with the lattice type. For a hexagonal lattice,

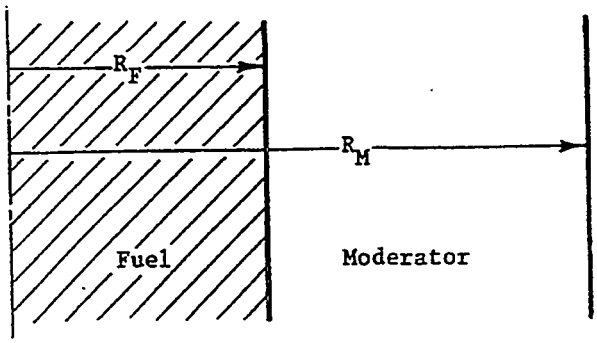
$$\alpha = \frac{\sqrt{3}}{2} \text{ and } \tau_0 = 0.12 .$$

3. Cylindrical Cell Using Sauer's Approximation[6] for the Dancoff Correction in a Square Lattice (ISSOPT = 2 or 1002)

   This option is identical with case 2 except that the lattice parameters are given by

$$\alpha = 1.0$$
$$\tau_0 = 0.08$$

4. Symmetric Slab Cell (ISSOPT = 3 or 1003)



In this case, the mean chord length is given by

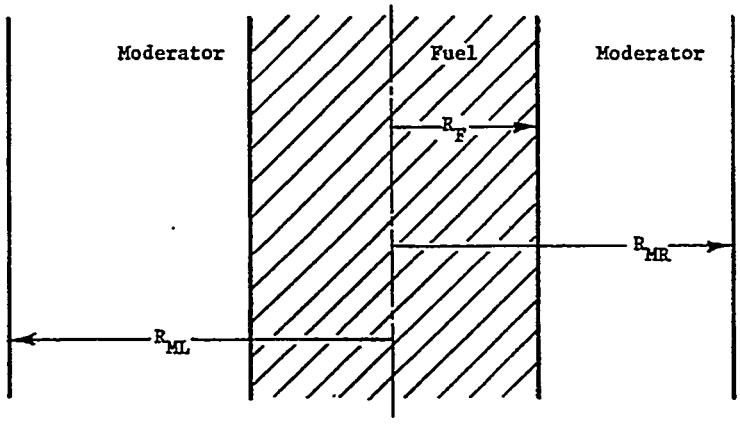
$$\bar{\ell} = 4R_F ,$$

and the Dancoff factor by

$$C = 2E_3 \left[\Sigma_M \left(\frac{V_M}{V_F} \frac{\bar{\ell}}{2} \right) \right] ,$$

where E_3 is the E_3-exponential function.

5. Asymmetric Slab Cell (ISSOPT = 4 or 1004)



In this case, a slab fuel region is surrounded on either side by moderator regions of differing thicknesses and/or compositions. The mean chord length in the fuel is given by

$$\bar{\ell} = 4R_F ,$$

where there are now two Dancoff factors, C_L and C_R, for the left and right sides, respectively. These values are calculated as for the symmetric slab case, and a "total" Dancoff factor is derived from

$$C = \tfrac{1}{2} (C_L + C_R) .$$

6. Isolated Lump (ISSOPT = 5 or 1005)

For this case, there is no "shadowing" of the fuel lump due to the other lump; hence, C = 0.0. There is, however, an effective escape cross section, $\sigma_e = 1/\bar{\ell}$, which must be included in the σ_0 term of the Bondarenko calculation. The $\bar{\ell}$ is geometry-dependent and is given by

a. $\bar{\ell} = 4R_F$ (slabs)

b. $\bar{\ell} = 2R_F$ (cylinders)

c. $\bar{\ell} = 4/3R_F$ (spheres)

7. Cylindrical Cell-Bell Approximation (ISSOPT = 6 or 1006)

This approximation is analogous to option 2 above (ISSOPT = 1), but uses a different expression for C:

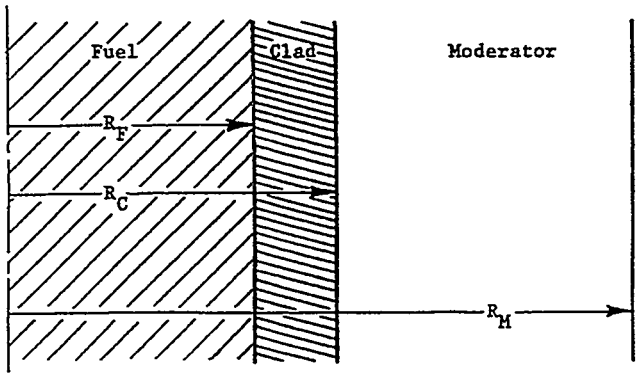
$$C = \frac{1}{1 + \Sigma_M \bar{\ell} \frac{V_M}{V_F}} .$$

The $\bar{\ell}$ term is determined as in 6 above.

8. Symmetric Slab Cell-Bell Approximation (ISSOPT = 7 or 1007)

This approximation is analogous to case 6, except that it is for slabs instead of cylinders. The same expression is employed to calculate a Dancoff factor, using appropriate values for $\bar{\ell}$ and for volumes.

9. Cylinder Cell Using Sauer's Approximation for a Hexagonal Lattice and Including Cladding Effects (ISSOPT = 8 or 1008) per the Williams and Gilai prescription[7]



In this case, one follows the procedures for option 2 (ISSOPT = 1). The Dancoff factor for no clad is then modified by multiplying by

$$(1 - P_c)^2 ,$$

where P_c is the clad collision probability and is derived from Sauer's expression for the escape probability of a hollow cylinder:

$$P_{esc} \sim \frac{1}{\Sigma\bar{\ell}} \frac{\left(1 + \frac{\Sigma\bar{\ell}}{n+1}\right)^{n+1} - 1}{\left(1 + \frac{\Sigma\bar{\ell}}{n+1}\right)^{n+1}},$$

where Σ and $\bar{\ell}$ are the total cross section and mean chord length of the clad and n is a geometry-dependent factor presented in Sauer's article.

Williams and Gilai[7] have parameterized n by

$$n = 3.58 + 0.4\chi + 3.5\chi^2, \chi \leq 0.4$$

$$= 0.474 + 15.057 - 13.73\chi^2, \chi > 0.4,$$

where χ is the ratio of the inner to outer radius of the clad.

The escape probability is related to the collision probability by

$$P_c = \bar{\ell}\ \Sigma P_{esc},$$

where $\bar{\ell}$ is 4V/S for the cladding region.

10. Cylindrical Cell Using Sauer's Approximation for a Square Lattice and Including Cladding Effects (ISSOPT = 9 or 1009)

The procedure is exactly as for case 9 (ISSOPT = 8), except that the lattice constants from option 3 (ISSOPT = 2) are used.

F1.2.2 EQUIVALENT HETEROGENEOUS LEAKAGE CROSS SECTION

In all cases, the Dancoff factors are used in an expression that gives an equivalent heterogeneous cross section that accounts for leakage and lump-to-lump interaction effects:

$$\Sigma_H = \frac{(1 - C)A}{\bar{\ell}[1 + (A - 1)C]},$$

where A is a geometrically dependent correction factor to account for error in the use of the Wigner rational approximation to calculate the escape probability from the lump. In BONAMI, expressions developed by Otter[8] are used which are cross-section and geometry-dependent and which essentially force the Wigner escape probability to agree with the exact escape probability for the particular geometry by determining a value of A as a function of $\Sigma_T\bar{\ell}$ for slab, cylindrical, or spherical geometries.

F1.2.3 TOTAL CROSS-SECTION ITERATION

BONAMI allows the user to specify whether or not the code will iterate to determine the effect of σ_0 values from previously shielded total cross sections for all groups and zones in the problem. In the noniterative situation, BONAMI uses the potential scattering cross sections in the determination of the σ_0 value.

F1.2.4 ESCAPE CROSS SECTIONS FOR MODERATOR REGIONS

In two-region cell analyses such as those used for the bulk of the Dancoff options discussed previously, the end result is to determine an escape probability for the fuel region which is used to infer an escape cross section for the fuel region. Commonly, escape effects for the moderator are ignored. This situation arises for several reasons, including the fact that escape effects from the moderator can be ignored safely for a large class of problems coupled with an increased geometrical complexity for the typical moderator region (e.g., the moderator may be in an annular or shell region).

In some codes, the approach is to ignore moderator escape effects and to treat the moderator separately in a smeared homogeneous mockup of the entire cell, while the fuel region uses Dancoff-type analyses such as those above. In TDOWN,[3] the approach is more correct and rigorous: a discrete-ordinates calculation is available for determining escape probabilities for all zones in a system, and these are used to infer "escape cross sections" in a consistent manner for all zones.

BONAMI uses a reciprocity relationship to determine its moderator values. For a two-region system, we can write

$$\Sigma_1 P_{1\to 2} V_1 = \Sigma_2 P_{2\to 1} V_2 ,$$

where Σ_1, Σ_2 are total cross sections for the two regions; V_1, V_2 are the volumes; and $P_{1\to 2}$, $P_{2\to 1}$ are the probabilities that a neutron born in one of the regions will make its next collision in the other region.

We assume that the moderator escape probability, $P_{2\to 1}$, can be expressed in a rational form:

$$P_{2\to 1} = \frac{\Sigma_{2e}}{\Sigma_2 + \Sigma_{2e}} .$$

Since all terms in the reciprocity equation are known except $P_{2\to 1}$, this term is determined, leading directly to a value of the moderator escape cross section, Σ_{2e}.

F1.2.5 SELF-SHIELDED TRANSFER MATRICES

BONAMI has provisions for self-shielding the individual elements in a transfer matrix, even for the higher-ordered Legendre coefficients. The formats and schemes used for the "transfer" arrays are exactly the same as for the 1-D cross-section data. This task is accomplished as follows:

In an AMPX master library, transfer matrices are structured in a sink-group ordered arrangement:

Word describing which groups scatter to a group

Scatter to the group from the first group designated

.
.
.
.

Only nonzero terms are generally included

Scatter to the group from the last group designated

Word telling which groups scatter to the next group

Scatter to the group .....

.
.
.
.
etc.

The format of the Bondarenko data uses six words to describe the information for a particular process:

1. MT, an identifier for the process (e.g., 1 for total, 2 for elastic scattering, etc.)

2. NF, the first group that has Bondarenko data.

3. NL, the last group that has Bondarenko data.

For 1-D data, the fourth, fifth, and sixth parameters are zero. For two-dimensional (2-D) transfer matrix data, these parameters are used as follows:

4. Order of Legendre coefficient.

5. Offset (from the magic word) within the scattering terms to a group of the term for which the Bondarenko data apply. The magic word is a word defining the number of terms supplied to determine the "in-scatter" source to a group.

6. Zero.

The latter three parameters are not used during the iteration part of the Bondarenko procedure, but only when the shielded values are parceled out to their assigned positions. The use of this strange arrangement is justified by the following arguments.

1. The basic iteration does not think about transfer matrices. This procedure allows simplification and takes less core than it would to carry "transfer matrix" structured Bondarenko factor arrays.

2. The schemes are general enough to handle any foreseeable situation.

3. Elastic scattering is generally the only scattering process that will be self-shielded. For the heavy nuclides, with most group structures, the transfer matrix needs a within-group term and one downscatter term. This fact suggests that it is enough to include only the Bondarenko factors for the within-group term, since the downscatter value is readily obtained by subtracting the within-group from the shielded elastic value.

BONAMI makes the transfer matrix substitutions as directed by the available data. This step may leave a portion of the transfer matrix unshielded, in which case BONAMI will normalize those terms to the difference between the shielded elastic value (or other process) and the sum of the shielded terms. The corresponding terms in the P_ℓ ($\ell > 0$) matrices are multiplied by the same factor as used for the P_0 terms.

F1.3 INTERPOLATION SCHEME

A large part of the testing of BONAMI involved running identical cases on alternative codes and comparing cross-section values. These tests revealed alarming variations in individual cross sections which finally led to a detailed study of procedures used to interpolate in tables of Bondarenko factors.

When confronted with the need for interpolating within a table of values for a function of great or unknown complexity, there is a real temptation to use the well-known Lagrangian interpolation schemes. The reasons are simple: the scheme is easy to apply; all points in the tabulation are reproduced; all points can contribute to the final polynomial, which represents the function. The original BONAMI code, SPHINX,[2] and EPRI-CELL[9] all use this approach. However, a careful examination of the codes will reveal that all have encountered problems with the scheme.

The problems are vividly illustrated in Fig. F1.3.1, where we show the effects of varying the order of Lagrangian fit to a typical tabulation of factors. In this figure, only a small portion of the total range is shown (the curve is for one temperature and had six values of σ_0). The ordinate is transformed to a log σ_0 scale as is commonly done because of the widely varying magnitudes of the σ_0 values which are taken, for example, at σ = 1, 10, 100, ...10^8. (Note that it is this transformation which yields the familiar "S-shape" to the curves. The bottom of the S is due to the fact that the log scale cannot accommodate negative σ_0 values and the cross section does not vary much between values of σ = 0 and σ = 1.)

Several problems are immediately apparent. First, and most significant, is that the curves do not converge with increasing order. Second, the curves are not all monotonic, and, third, there is the very real possibility of a discontinuity caused whenever the interpolation scheme shifts from one set of points to another set (cf., the third-order curve).

As mentioned previously, BONAMI, SPHINX, and EPRI-CELL have all encountered problems with Lagrangian schemes and have taken action to circumvent the problem.

In the case of SPHINX, it is noted that there is a mechanism for avoiding the higher-order fits which are most troublesome. Also, since any of the polynomial fits above linear (order 2) can be nonmonotonic, the developers have caused the code to take on the end point values in a panel for those cases where the functions stray above and below the panel end values.

EPRI-CELL transforms the factors to a smoother function,

$$F_g(\sigma_0,T) = \sqrt{\sigma_0}\, e^{-\frac{1}{2} f(\sigma_0,T)},$$

and uses fourth-order interpolation. This apparently avoids many of the difficulties, but it is not obvious that the fits will not still exhibit a nonphysical nonmonotonic behavior in some cases.

BONAMI avoids the problem by changing to nonLagrangian schemes, as described below.

In arriving at our scheme, several alternative approaches were examined.

The empirical schemes of Kidman,[10] used in ETOX,[11] are attractive and are based on the use of the tanh function:

$$f = A \tanh(B\sigma_0) + C$$

for σ_0 interpolation. The constants A, B, and C can be adjusted to give the "S-shape." This method was never tried in BONAMI, primarily because our studies discovered a new and very consistent method for interpolating, as will be described below.

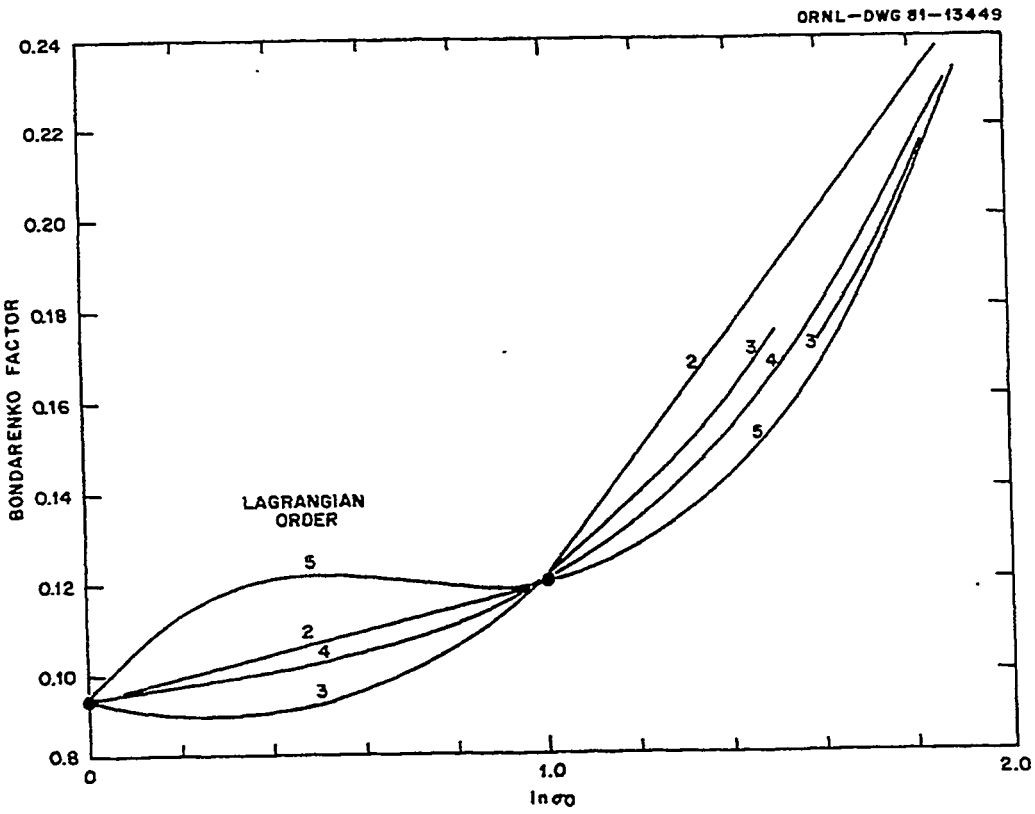


Figure F1.3.1 Effects of varying the order of Lagrangian interpolation with typical Bondarenko factor tables

Another very attractive scheme for σ_0 interpolation was suggested by M. Segev in a June 20, 1979, letter to J. Kallfelz, C. Weisbin, and M. Williams at ORNL, who noted that if a resonance is all contained in a group, and, if one ignores Doppler broadening, the zero-temperature average cross section based on the NR approximation is analytic. The resulting analytic expression can be used to interpolate in tables of Bondarenko data yielding an expression of the form

$$F(\sigma) = \sqrt{\frac{F_1^2\ 1-F_2^2\ \sigma_2 - F_2^2\ 1-F_1^2\ \sigma_1 + F_2^2-F_1^2\ \sigma}{1-F_2^2\ \sigma_2 - 1-F_1^2\ \sigma_1 + F_2^2-F_2^1\ \sigma}},$$

where the point, σ, is in the interval (σ_1, σ_2) and the factors are (F_1, F_2). Based on the nice behavior of this form in a simple test program, this scheme was introduced into BONAMI to replace the Lagrangian scheme. Problems were immediately encountered. As long as F_1 and F_2 are less than 1, one can show the scheme to be monotonic, such that one will not violate the bounds of the values in the table. When either F_1 or F_2 goes larger than 1, however, the values can, and do, vary without bound. This is understandable, when one examines the basis of the above equation. It is absolutely based on Bondarenko factors which are upper-bounded by 1.0, since Doppler broadening is neglected. With the typical energy group structures at ORNL, however, it is very common to find several groups within a single resonance, and, in this case, the Bondarenko factors can be greater than 1.0.

To augment the Segev scheme for σ_0 interpolation, a new method was developed for temperature interpolation. Consider Fig. F1.3.2. Five curves of Bondarenko factors are shown with points at T = 300, 900, and 2100 K. Each curve is for a fixed value of σ_0. If the behavior of f with T were linear, the three points on each curve would fall in a straight line on a linear scale. Examination reveals that the curves at the bottom do exhibit this behavior, with increasing degrees of departure as the value of f increases. If, on the other hand, we shift to a different scale (e.g., the $\sqrt{T}$ scale, we can fix the ends and determine where the $\sqrt{900}$ would fall. If f is linear in $\sqrt{T}$, one would then find the points on a straight line in this reference system. What this does, of course, is shift the middle point to the right relative to the 300 and 2100 K points. As illustrated, some curves are fit better, while the "linear" curves are not. Continuing, a shift to a ln T scale is better for large f, but worse for others. Unfortunately, there are situations for which none of these schemes are good, and there are always the "in-betweens." This realization led to the consideration of a monotonic scheme, such that a curve could always be found to fit three monotonic points. One such scheme is to write

$$f(T) = f_i + \frac{T^p - T_i^p}{T_{i+i}^p - T_i^p}\,(f_{i+1} - f_i)$$

for the temperature variation. Here p is a constant determined to fit three points in a curve. Figure F1.3.3 shows a typical fit of three points using this scheme.

This scheme has many advantages: it is general, it is compact, and it is relatively simple. The values for p can be determined as they are needed in a straightforward fashion (though it would be nicer if they were supplied as part of the data). For the temperature variation of three curves, the p can be accommodated for no storage penalty, since the 900 K curve is explicitly determined from the p value and the 300 and 2100 values (i.e., to store p values, one can replace the 900 curve).

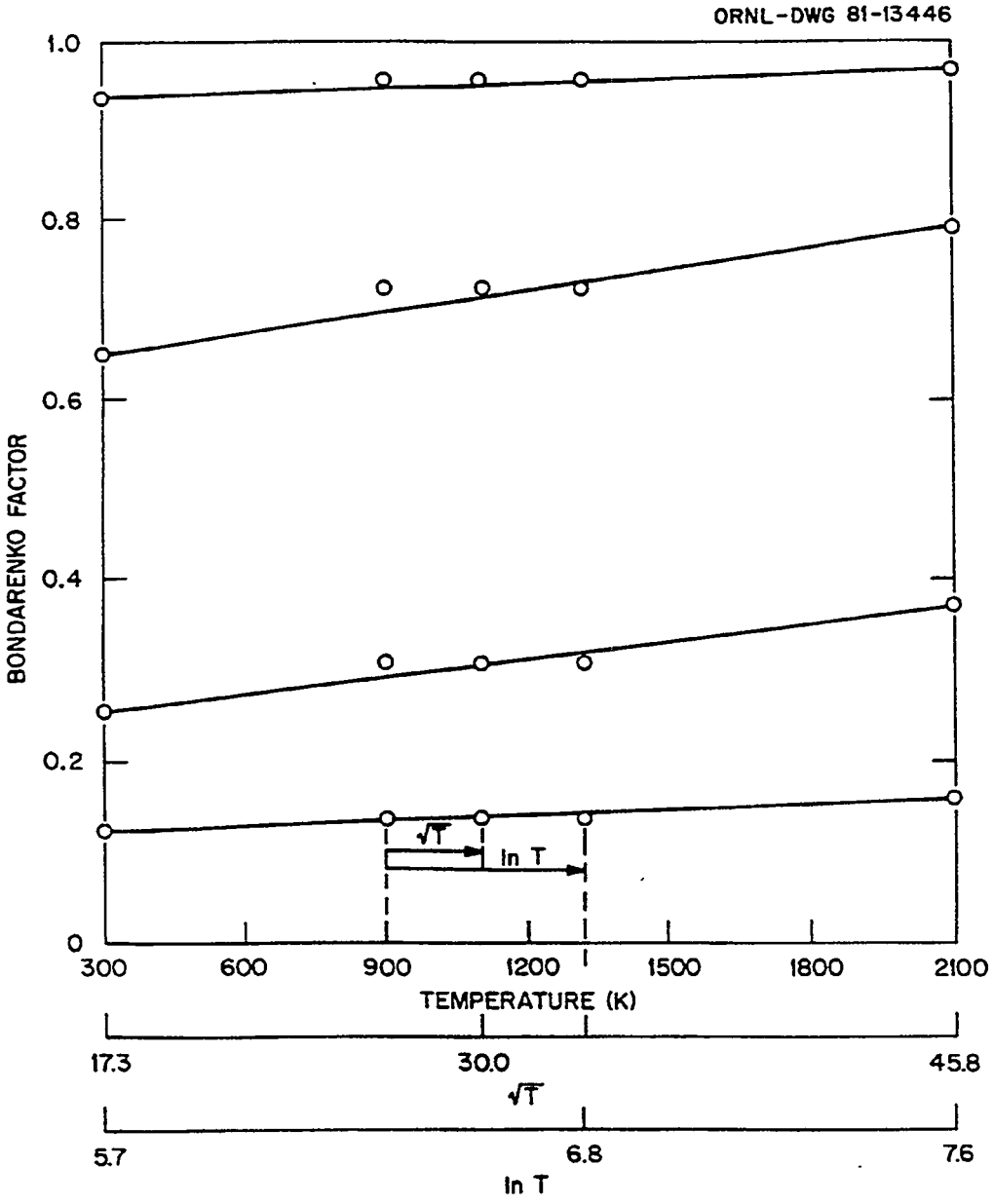


Figure F1.3.2 Temperature variation of Bondarenko factors plotted on three overlaid scales

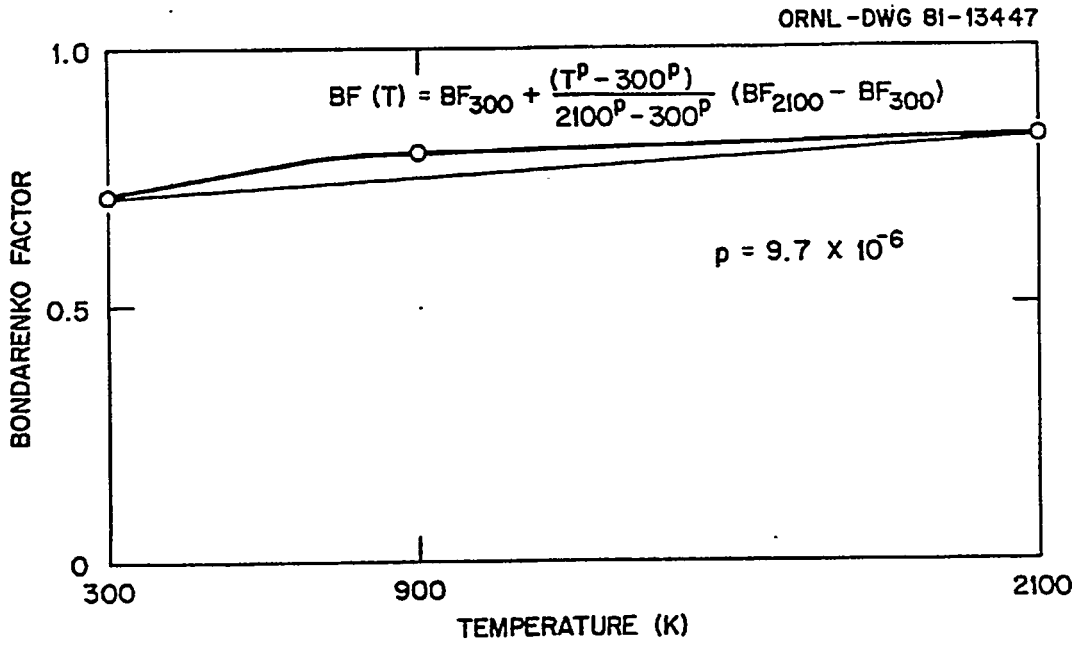


Figure F1.3.3 Typical fit to the temperature variation of Bondarenko factors with this method

Because of its success for temperature interpolation, it was decided to try to use it for the σ_0 variation. In this case, the scheme was to interpolate each curve for each σ_0 of each group of each process to the temperature requested. This new curve was then "fit" with other powers which were carried to the iteration calculation:

$$f_T(\sigma_0) = f_T(\sigma_i) + \frac{\sigma_0^q - \sigma_i^q}{\sigma_{i+1}^q - \sigma_i^q}\left[f_T(\sigma_{i+1}) - f(\sigma_i)\right].$$

This scheme was introduced into BONAMI and compared with alternative methods. Difficulties were noted arising primarily from the fact that for a step function it is crucial which three points one uses to determine the monotonic power fit. Consider the typical "S-shape" Bondarenko behavior shown in Fig. F1.3.4. One can use the three-point scheme described for temperature to determine a q for a region. In this case, points 1,2,3 could be used to determine a q for panels 1–2 and 2–3; 2,3,4 would give a q for panel 3–4; 3,4,5 for panel 4–5; and 4,5,6 for 5–6. However, within the five panels shown, the three interior panels are also members of one other equally close three-point panel (e.g., 2–3's q could be determined from 2,3,4). The major problem is for 3–4, where the two three-point regions can define either a concave or convex monotonic curve.

The power q can be treated as a point function rather than a constant panel value, and, as will be shown below, this method circumvents much of the problem. Figure F1.3.5 illustrates the expected behavior caused by varying the powers in a panel. Assume that the interpolation scheme is now expressed by

$$f(\sigma) = f(\sigma_1) + \frac{\sigma^{q(\sigma)} - \sigma_1^{q(\sigma)}}{\sigma_2^{q(\sigma)} - \sigma_1^{q(\sigma)}}\left(f(\sigma_2) - f(\sigma_1)\right),$$

where

$$q(\sigma) = q(\sigma_1) + \frac{\sigma - \sigma_1}{\sigma_2 - \sigma_1}\left(q(\sigma_2) - q(\sigma_1)\right).$$

By allowing p to vary with x (or σ), we can move *between* the various monotonic curves on the graph *in a monotonic fashion*. Note that when p crosses the p = 1 curve, the shape changes from concave to convex, or vice versa. This shape change means that we can use the scheme to introduce an inflection point, which is exactly the situation needed in panel 3–4 of Fig. F1.3.5. Figures F1.3.6 and F1.3.7 show typical "fits" of the factors using the new scheme. Note, in particular, that since this scheme has guaranteed monotonicity, it easily accommodates the end panels which have the smooth asymptotic variation.

This new scheme has been used in BONAMI with apparent success. Even considering the extra task of having to determine the powers for temperature and σ_0 interpolation, the method is not significantly more time-consuming than the alternative schemes.

Note that there is nothing in this method which ties it to Bondarenko processing. It has been successfully used for a variety of other situations where a simple, monotonic variation is desirable.

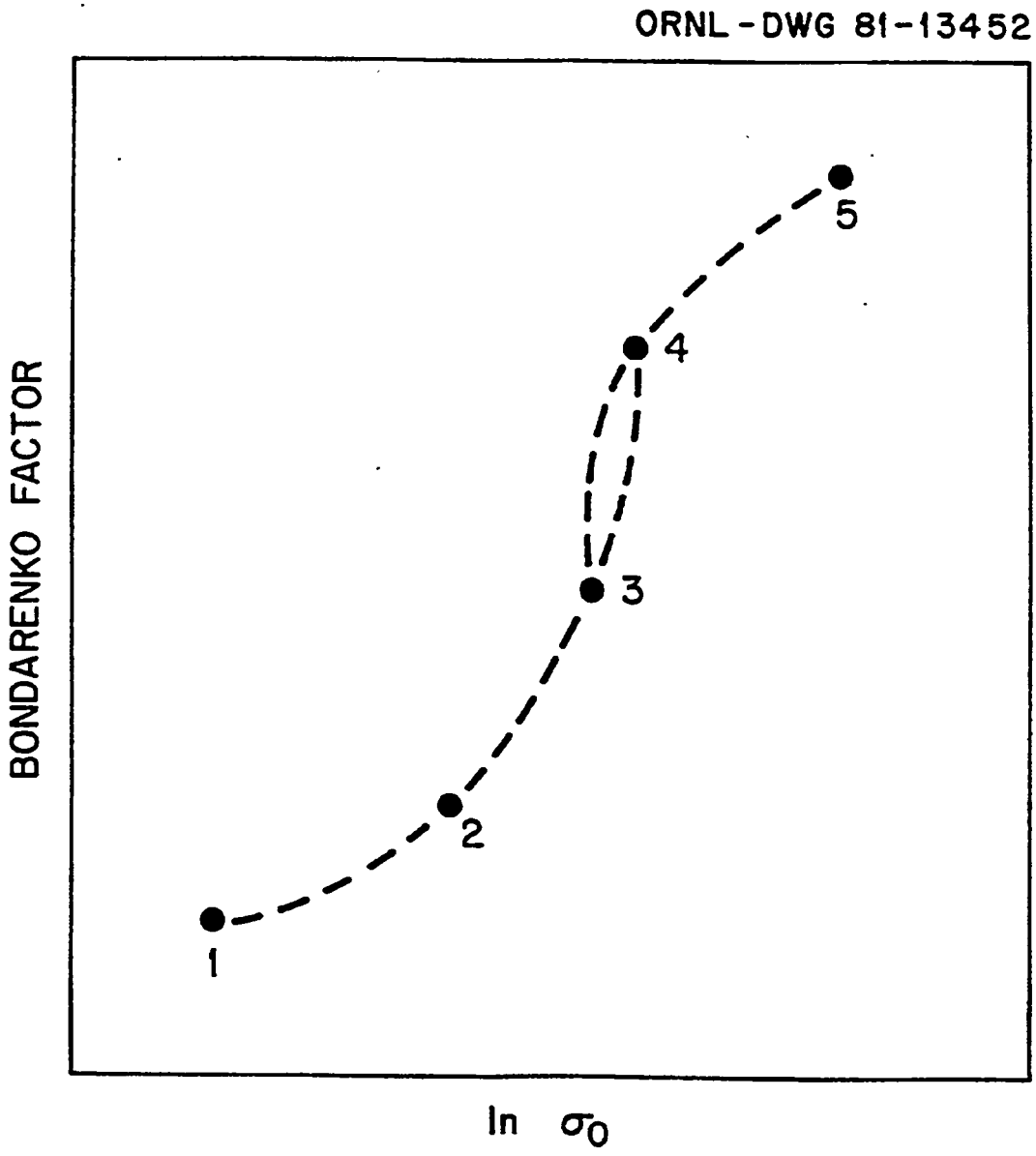


Figure F1.3.4 Typical "S-shape" of σ_0 variation of Bondarenko factors

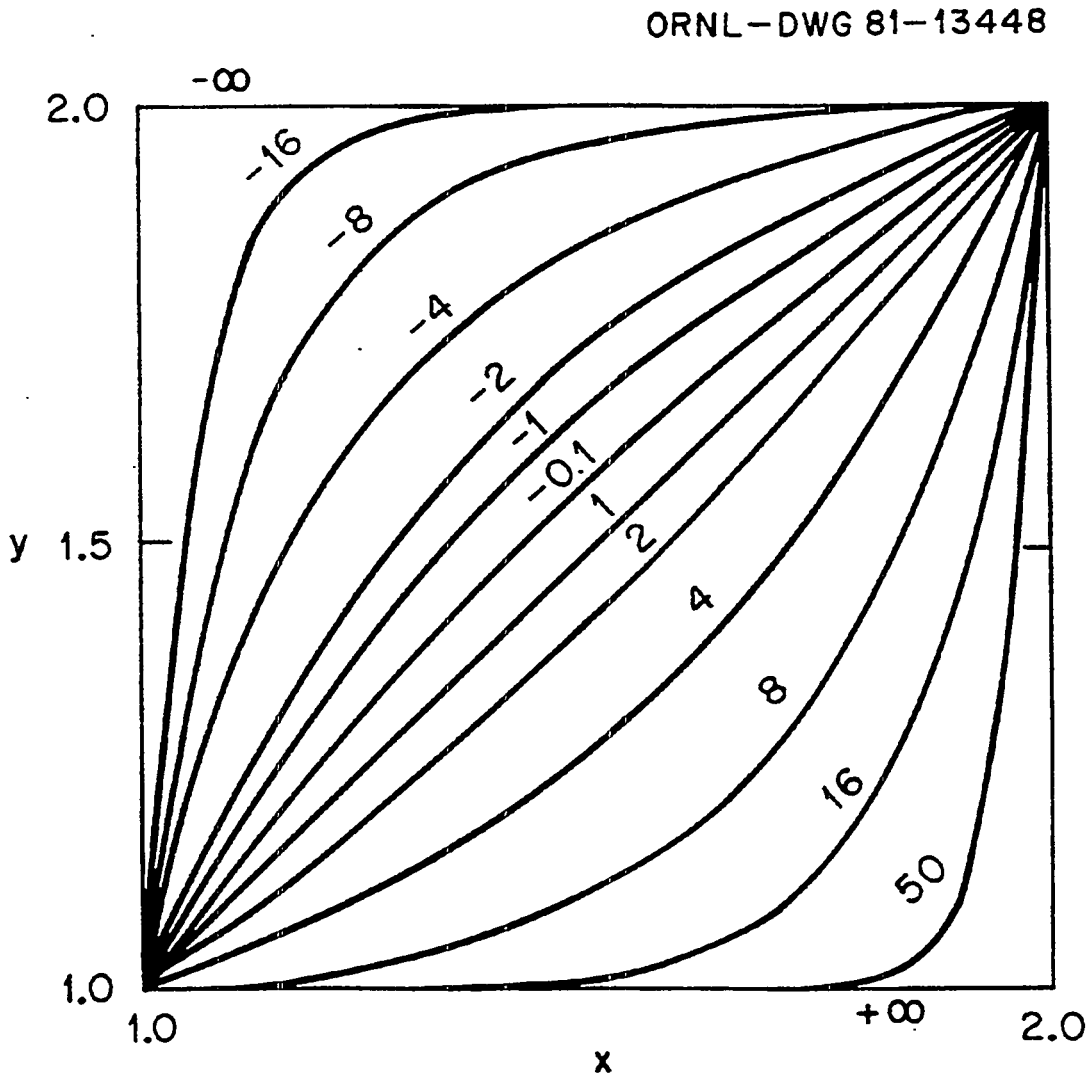


Figure F1.3.5 Illustration of the effects of varying "powers" in the new interpolation method

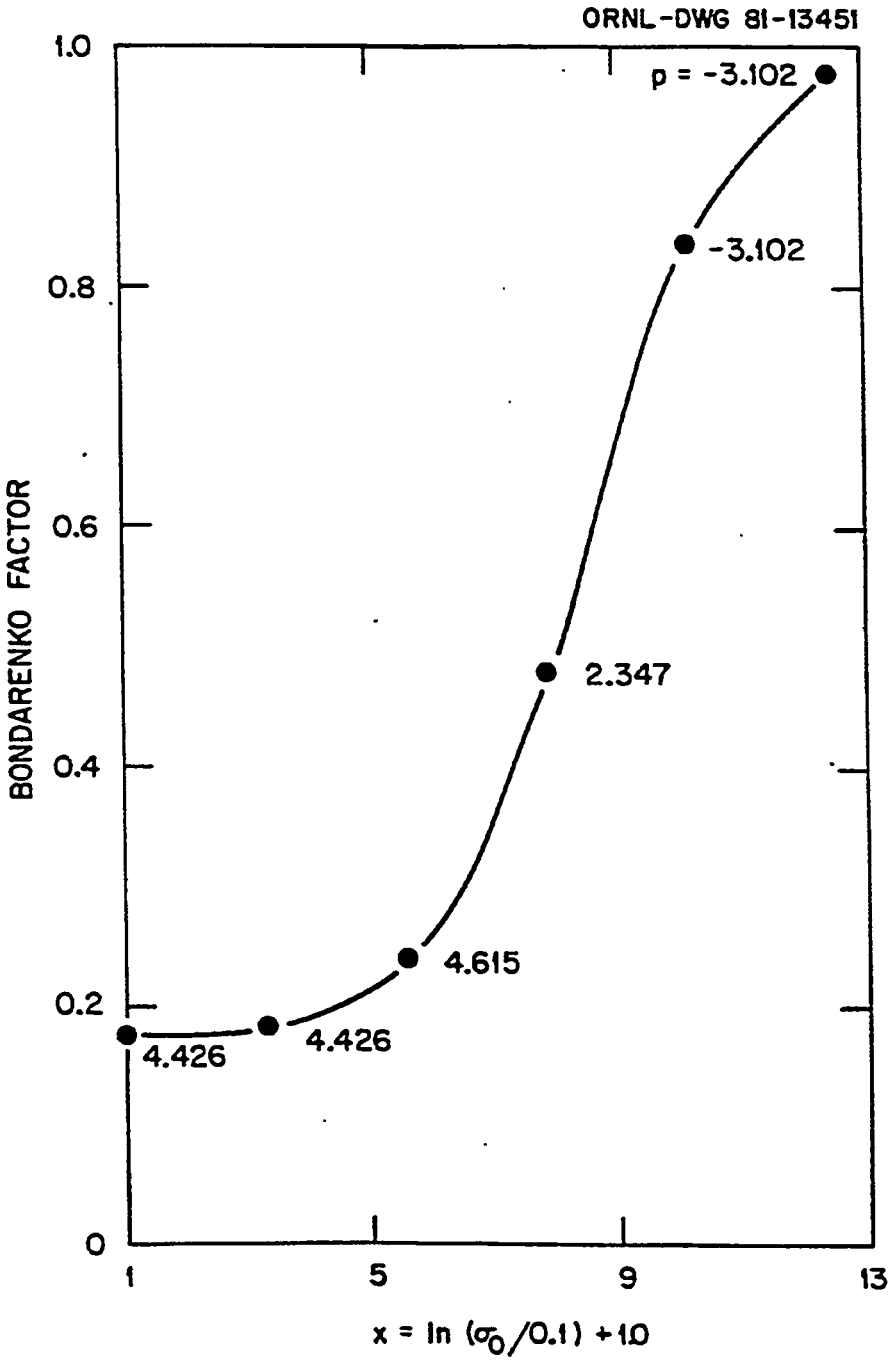


Figure F1.3.6 Example 1: use of new method to fit the σ_0 variation of Bondarenko factors

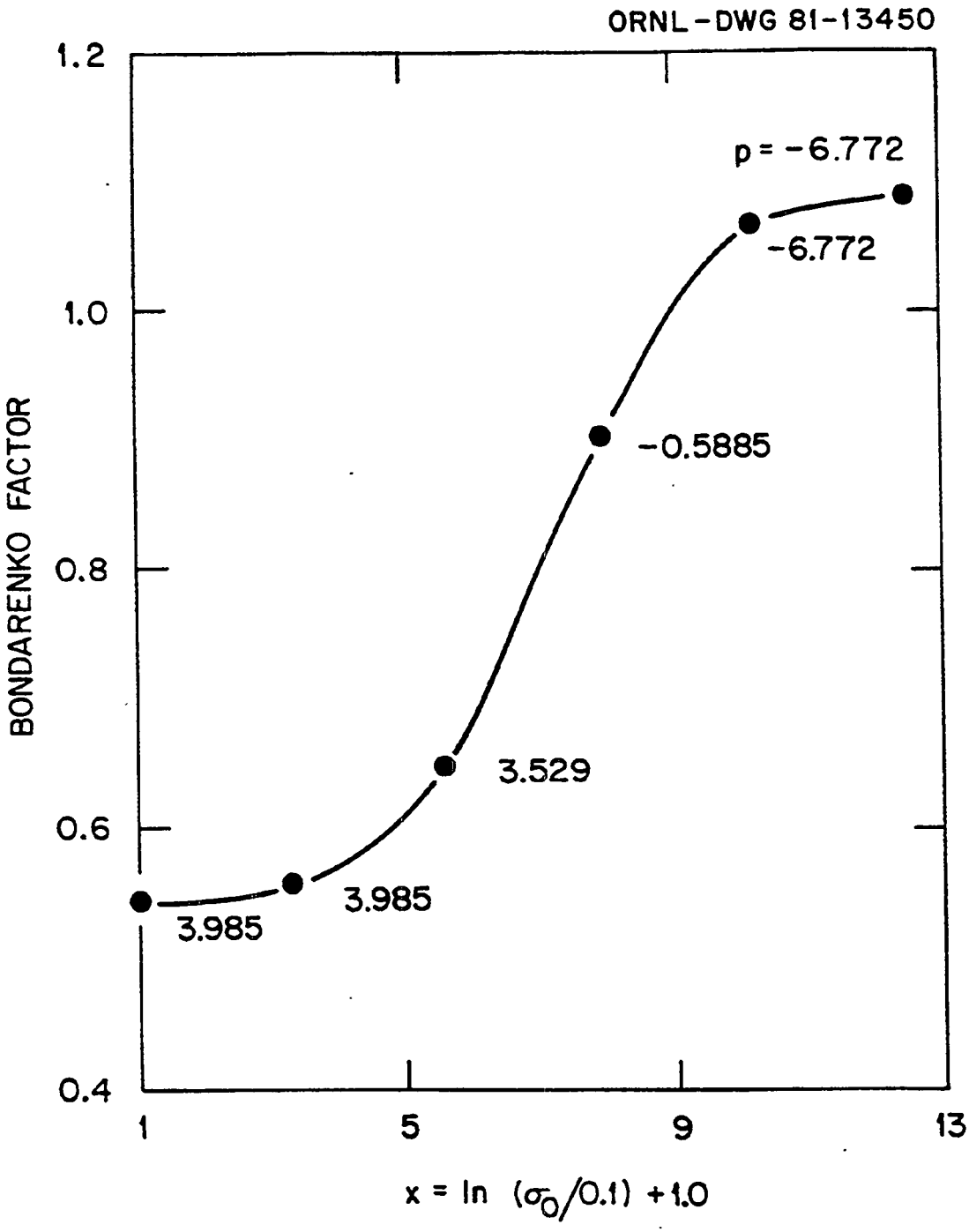


Figure F1.3.7 Example 2: use of new method to fit the σ_0 variation of Bondarenko factors

F1.4 PROGRAMMING DETAILS

The flow chart for BONAMI is very simple and is shown in Fig. F1.4.1. With the exception of "library routines," which are shared by many of the modules in the AMPX[1] system, BONAMI consists of approximately 1800 cards. The subroutines in the program are listed below, along with a brief description of their intended purpose.

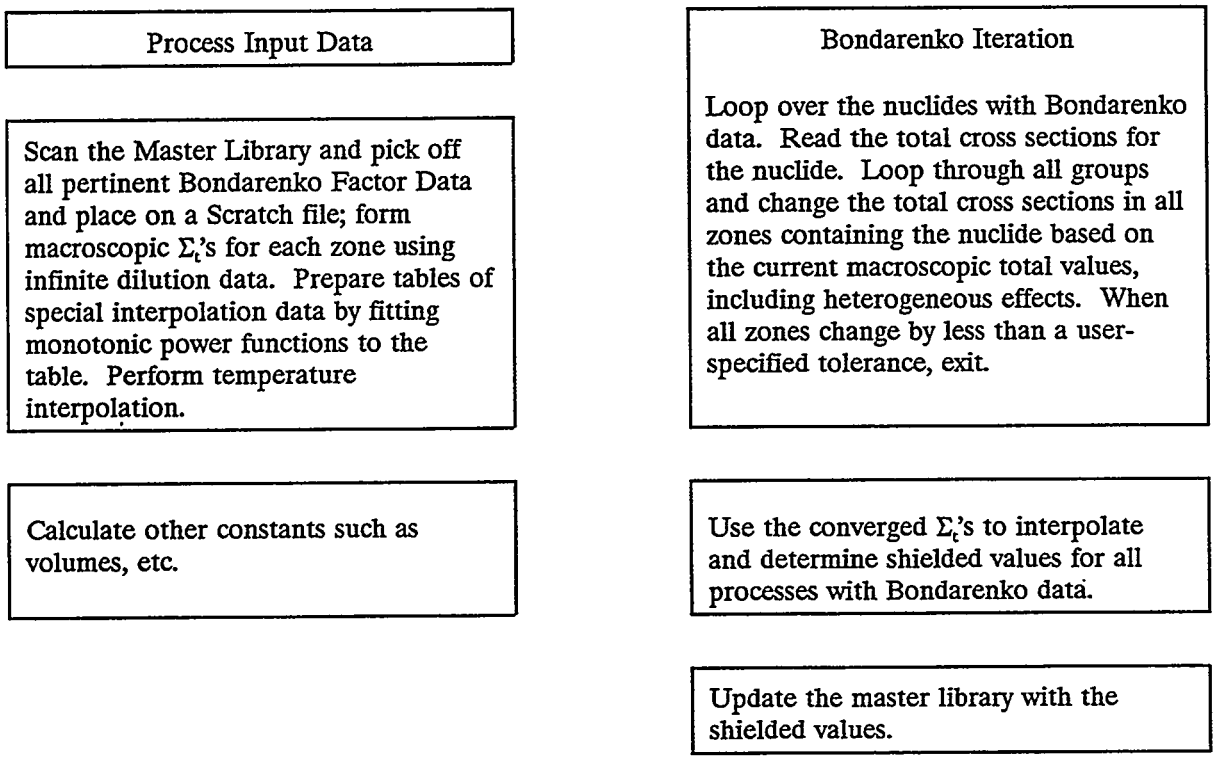


Figure F1.4.1 BONAMI calculational flow

F1.4.1 SUBROUTINE DESCRIPTIONS

On the following pages is a functional description of the subroutines in BONAMI. The main routines are listed in roughly the order in which they are accessed in a typical run. Following this, the remaining routines are listed in alphabetical order.

MAIN Program

This routine sets a parameter, IEXCT, to zero for running in AMPX or to 1 when it is used in the SCALE system. This is the only difference between BONAMI and BONAMI-2.

Call START to start calculation.

Subroutine START

Assign default values for input parameters.

Call MESAGE to print out case header page.

Call FIDAS or QOREAD to read first block of input data.

Open all I/O buffers.

Call ALOCAT to dynamically allocate core space to subroutine BOND, based on core region for the job.

Call CLOSDA to release logicals N8 and N9 for use in later modules.

Subroutine BOND

This routine controls the overall flow of a BONAMI calculation.

Set up array pointers in container array, D.

Edit Block 1 input data.

Call FIDAS or QOREAD and read remainder of input data.

Call FIXMIX and make adjustments to mixing table input parameters, if required.

Call EDIT and edit remainder of input data.

Set up array pointers for Bondarenko calculation.

Call TOCM to read table of contents from master library and determine maximum sizes of cross-section blocks that will be read.

Call I/O to read energy group boundaries.

Call MAST to read Bondarenko factors for nuclides required in the problem.

Call GEOM to determine geometrical constants – volumes, average chord lengths, etc. – which will be required.

Call MIX to produce pre-iteration macroscopic total cross sections.

Call VEDIT to edit geometrical data.

Call ARENKO to perform Bondarenko iteration.

On Option Call BFEDIT to produce edits of final shielded cross sections and/or Bondarenko factors for each nuclide in problem.

Call TABLE to produce a "Table of Contents" for output master library that includes all multiple sets, etc.

Call TUB to write "Table of Contents" onto new master library.

Call GEORGE to write energy structure arrays onto new master library.

Call MASTER to write remainder of new master library.

Call RECTRY to ensure consistency of "Table of Contents" on new master library with actual data that were written by subroutine MASTER.

Subroutine ARENKO

This routine performs the Bondarenko iteration.

Call OPENDA and initialize direct-access space on logicals N8 and N9, based on actual problem needs.

Call PRTIME to edit time.

Call XSEDIT to edit pre-iteration macroscopic total cross sections.

Go into iteration loop.

Determine effective escape cross sections for zones in system based on input.

Call DANCOF to determine Dancoff factors.

Go into loop over nuclides with Bondarenko data.

Read Bondarenko factors for nuclide.

Go into loop over energy groups with factors.

Determine σ_0 for nuclide based on current values of cross sections.

Interpolate in Bondarenko factor tables.

Produce new values for total cross section and update macroscopic total values.

End loop over groups.

Call RITE to write σ_0 values to unit N9.

End nuclide loop.

Determine if more iterations are required based on convergence tests of macroscopic total cross sections by zone.

Edit iteration statistics.

End iteration loop.

Call XSEDIT to edit final values of macroscopic total cross sections.

Go into loop over all processes for nuclides with Bondarenko factors.

Read Bondarenko data for nuclide and process.

Call REED to read converged σ_0's for nuclide determined in iteration to interpolate and determine shielded cross sections.

Call RITE to write values onto scratch unit N8 for later access.

End nuclide/process loop.

Call XSEDIT to edit macroscopic "escape" cross sections.

Produce edits of Dancoff factors and related cross-section values for the problem.

Subroutine MASTER

This routine is to control the writing of the shielded cross sections on the output master library.

Loop over nuclides on original master library.

Determine if the nuclide

a. is required for this problem,
b. has multiple sets created, and/or
c. contains Bondarenko data.

If not required in problem, call CAPY and copy data directly to new master library.

If this set occurs in more than one zone in the problem, and, therefore, will create multiple sets call CAPY and write onto scratch unit MSC.

Loop over mixing table entries to determine how many times to copy set.

Call CAPY and read from original master or logical MSC (multiple sets) and replace cross-section values with new shielded values before writing onto new master library.

End mixing table loop.

End nuclide loop.

The remaining BONAMI routines are discussed in alphabetical order. Routines that are taken from the AMPX general-purpose library (used by many modules) will be listed following these subroutines.

Subroutine BFEDIT

This routine produces edits of cross sections and/or Bondarenko factors for nuclides in the problem. It contains calls to REED to read pertinent data from logical units N8 and N9, which were written in ARENKO.

Subroutine BTERP

This routine serves to interpolate in tables of numbers using the interpolational scheme described in Sect. F1.3 of this report.

Subroutine CAPY

This routine is used to copy all the cross sections for a nuclide from logical N1 to logical N2. Optionally, cross-section values are replaced with shielded values, for those nuclides with Bondarenko factors. Many calls are made to IO and IO4 to read and write data, and to REED to obtain self-shielded values determined in ARENKO. For the case where cross sections are replaced, calls will be made to the following:

a. FODGE, to determine where the total, absorption, and capture cross sections are situated in the 1-D arrays;

b. FUDGE, to replace 1-D values with shielded values;

c. FACTOR, to determine values to multiply transfer elements by to ensure transfers sum to shielded total value for process in the case in which no transfer elements are replaced;

d. FUCTOR, to determine value by which to multiply unreplaced transfer elements to ensure transfers sum to shielded values;

e. STUFF, to replace transfer elements with shielded values; and

f. NORMAL, to normalize the transfer matrix based on factors determined in FACTOR or FUCTOR.

Function DANCOF

This routine determines Dancoff factors and, hence, escape probabilities and cross sections based on expressions discussed in Sect. F1.2 of this report. On option, it uses function OTTER to determine an accurate value of escape probability for slab, cylindrical, or spherical geometries. A function, E3, is sometimes called to evaluate the E_3 exponential function.

Subroutine EDIT

This routine produces edits of information primarily contained in Block 2 of the BONAMI input.

Function E_3

This function evaluates the E_3 exponential function.

Subroutine FACTOR

This routine determines values by which one should multiply elements in a transfer matrix in order to ensure consistency with the "total" shielded value. It is used for the case in which no factors are supplied for transfer matrix terms.

Subroutine FIXMIX

This routine is used to help ensure BONAMI can function with the input mixing table instructions. When possible, the routine will "fix" the mixing table.

Subroutine FODGE

This routine determines the locations in which the total, absorption, and capture cross sections are given in the 1-D cross-section tables. Its pointers are used by FUDGE.

Subroutine FUCTOR

This routine determines factors by which nonreplaced elements in a transfer matrix must be multiplied in order to ensure consistency with the "total" shielded values.

Subroutine FUDGE

This routine is used to replace 1-D values with their shielded values.

Subroutine GEOM

This routine determines volumes, average chord lengths, and other dimensions needed by the various heterogeneous options in BONAMI.

Subroutine GEORGE

This routine is used to copy energy group structures from the original library to the final library.

Subroutine GZONE

This is an experimental multizone treatment routine which will not be accessed by any of the options discussed in the input specifications of BONAMI.

Subroutine IDZONE

This function is used to construct new identifiers from a combination of the old identifier and zone number for cases where new identifiers are not supplied in the input.

Subroutine MAST

This routine reads data from the original master library, selects those nuclides in the problem, and calls routines that fit their Bondarenko data with the powers required by the special interpolation procedures described in Sect. F1.3 and writes these onto logical MSC. It also serves to select initial total cross sections for all nuclides in the problem. ROUGH is called to obtain the infinite dilution total cross-section values for nuclides with Bondarenko factors. SELECT performs the same service for nuclides without Bondarenko factors. NVERT may be called if the Bondarenko factors are supplied in the order of decreasing σ_0's. PCALC is called to fit just the temperature variation with powers. PXCALC interpolates the results from PCALC in temperature and fits these points with powers describing the σ_0 variation.

Subroutine MIX

This routine uses the mixing table to construct the initial macroscopic cross sections for each zone from the microscopic total values captured by the call to MAST. It also determines other cross sections needed by some of the Dancoff options.

Subroutine NORMAL

This routine uses factors determined in FACTOR or FUCTOR to normalize elements in the transfer matrices to ensure consistency.

Subroutine NVERT

This routine is called to invert the Bondarenko factor array in case it is supplied with high-to-low variation on σ_0.

Function OTTER

This routine contains expressions that will determine a geometry-dependent A-factor which can be used to correct the escape probabilities determined by the rational approximation.

Subroutine PCALC

This routine considers the temperature variation of the Bondarenko factors and uses the Newton root-solving technique to determine power fits to three-point panels in temperature.

Subroutine PXCALC

This routine starts by interpolating the information passed from PCALC to the problem temperature. This results in a series of 5- to 10-point curves in σ_0 for every group supplied for the process. These points are processed in monotonic groupings of three points to produce powers describing the σ_0 variation. Newton's method is used.

Subroutine ROUGH

This routine selects the infinite-dilution total cross sections for nuclides with Bondarenko factors. Optionally, it stuffs the potential scattering cross section for the nuclide into the total cross-section array for use with options where ISSOPT is greater than 1000.

Subroutine SELECT

This routine selects total cross sections from the 1-D tables for nuclides without Bondarenko factors. Optionally, it stuffs the potential scattering cross section for the nuclide into the total cross-section array for use with options where ISSOPT is greater than 1000.

Subroutine STUFF

This routine replaces individual elements in a transfer matrix in the case where these terms are self-shielded.

Subroutine TABLE

This routine is used to construct a "Table of Contents" for the master library BONAMI produces.

Subroutine TOCM

This routine scans the "Table of Contents" on the original master library to determine maximum array sizes that will be encountered in processing the data in the library.

Subroutine TUB

This routine writes the "Table of Contents" on the master library.

Subroutine VEDIT

This routine edits geometrical parameters, such as volumes, dimensions, etc.

Subroutine XSEDIT

This routine is used to edit macroscopic cross sections.

Subroutine ZZONE

This is an experimental routine for a special multizone treatment. This treatment will not be accessed by any of the options discussed in Sect. F1.5.

The remaining routines used by BONAMI are general-purpose routines that are shared by many AMPX modules.

Subroutine ALOCAT

This assembler routine is used to dynamically allocate core space to BONAMI. It calls BOND with two arguments, the array and its length in four-byte units.

Subroutine CLOSDA

This assembler routine is used to release a direct-access scratch file so that it can be reassigned, either as a sequential file or as a direct-access file with a different structure.

Subroutine COPY

This routine is used in conjunction with RECTRY to perform a final cleanup of the master library produced by BONAMI.

Subroutine FIDAS

This routine is used in conjunction with FFREAD to read the FIDO-formatted input data.

Subroutine FFREAD

This routine is used in conjunction with FIDAS to read the FIDO-formatted input data.

Subroutine FHLPR

This routine is used in conjunction with MESAGE to produce the header page, which precedes BONAMI printed output.

Subroutine INTIME

This routine is used in conjunction with PRTIME to produce edits of elapsed times during the calculation.

Subroutine IO

This routine is used to read or write short-list I/O records from sequential devices.

Subroutine IO4

This routine is used to read or write special transfer matrix directory records on an AMPX master library.

Subroutine MESAGE

This routine is used in conjunction with FHLPR to produce the header page, which precedes BONAMI printed output.

Subroutine OPENDA

This assembler routine performs the same service as the IBM "Define File" statement, which defines the structure of a direct access file.

Subroutine PRTIME

This routine is used in conjunction with INTIME to edit elapsed times throughout the course of a calculation.

Subroutine QOREAD

This routine is only used when BONAMI is used in SCALE. In this case, input data are read from a special binary file, as opposed to the FIDO-input card images.

Subroutine RECTRY

This routine is used in conjunction with COPY to perform a final cleanup of the master library written by BONAMI.

Subroutine REED

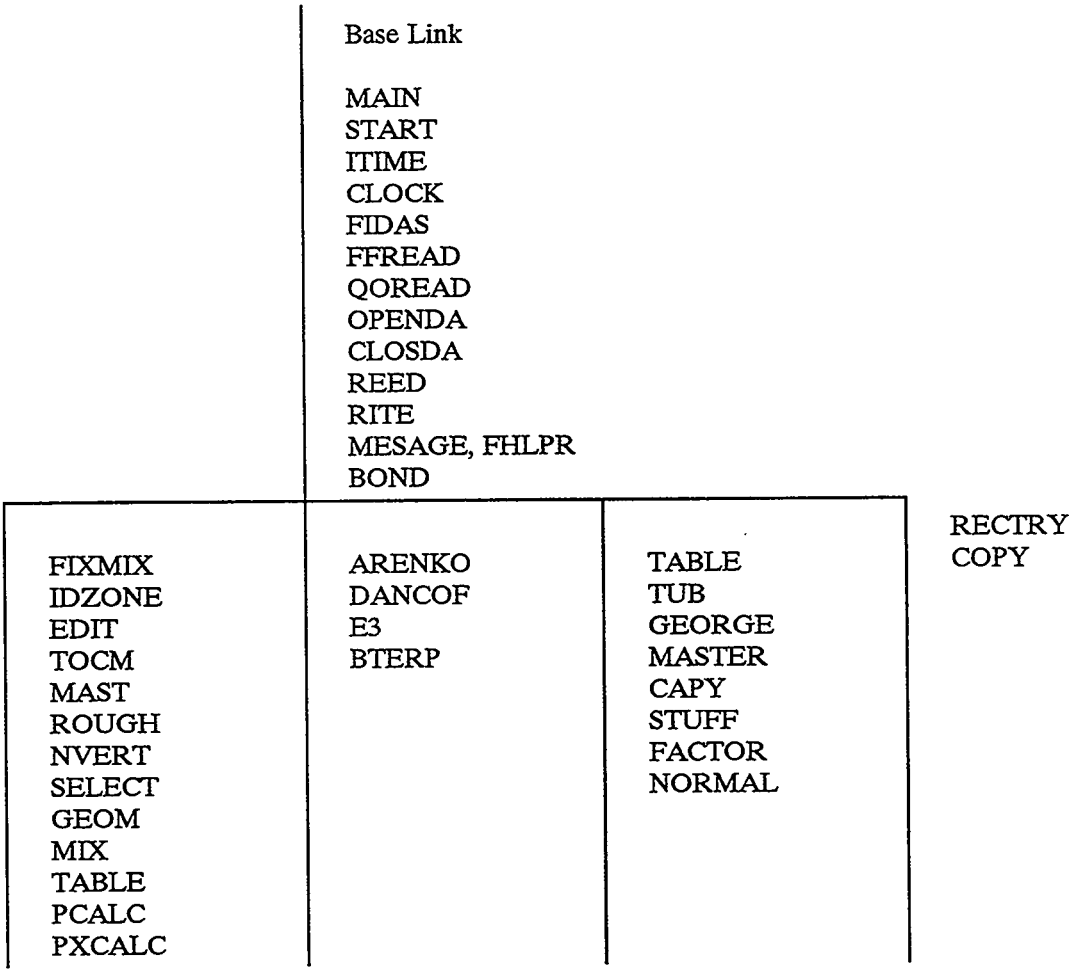
This assembler routine is used to read records from direct access units.

Subroutine RITE

This assembler routine is used to write records on direct access units.

F1.4.2 OVERLAY STRUCTURE

In most situations, BONAMI can be run without the use of an overlap structure, as it is relatively short. The following structure can be used in those instances when it is desirable to cut down on core requirements:



F1.4.3 NUCLIDE COPYING RULE

A programming quirk that has led to some confusion and minor problems with BONAMI is that the output library contains all data from the input library, even those nuclides which are not used in the Bondarenko calculation. In the event this is not desired, a simple AJAX[1] run can be used to select only the problem-related nuclides prior to the BONAMI case.

F1.4.4 INPUT/OUTPUT REQUIREMENTS

The following files are typically required by a BONAMI calculation:

Logical Unit	Use
5	Card Input
6	Standard Output
8	Direct Access Scratch Space
9	Direct Access Scratch Space
18	Scratch Space
19	Scratch Space
NEW (22)	Output Master Library
MMT (23)	Input Master Library
MWT (24)	Fitted Bondarenko Factors

The space requirements of logical 8 depend on the problem and will be that needed to hold all shielded cross-section values for all processes for all nuclides with Bondarenko data in the problem. For example, if the problem had two nuclides with 100 groups and each nuclide contained 10 processes, roughly $2 \times 100 \times 10 = 2000$ words would be needed. This amount of space must be less than or equal to the amount requested in the OPENDA call of the START routine. Because of certain "blocking considerations," a generous overestimation of space may be warranted (e.g., 20%).

Logical 9 will require roughly the same space as logical 8.

Logical 18 must be large enough to hold all data that will be written on the final output master library.

Logical 19 requires the amount of space needed to store one nuclide's cross sections or 50 words times the number of nuclides on the output master library, whichever is greater.

Logical 24 must be large enough to contain all Bondarenko factor data for all processes of all nuclides in the problem. This requires roughly the number of nuclides times the average number of processes times the number of groups times the number of temperatures times the average number of σ_0's words.

F1.5 INPUT INSTRUCTIONS

The input to BONAMI uses the FIDO schemes described in Sect. M10.

Block 1

0$ Logical Unit Assignments [4]
1. MMT – input master library (Default = 23)
2. MWT – scratch for Bondarenko factors (Default = 24)
3. MSC – scratch device (Default = 18)
4. NEW – output master library (Default = 22)

1$ Case Description [6]
1. IGR – geometry
   0 homogeneous
   1 slab
   2 cylinder
   3 sphere
2. IZM – number of zones or material regions
3. MS – mixing table length. This is the total number of entries needed to describe the concentrations of all constituents in all mixtures in the problem.
4. IBL – cross-section edit option (0/1 – no/yes)
5. IBR – Bondarenko factor edit option (0/1 – no/yes)
6. ISSOPT – Dancoff factor

ISSOPT	Option
0 or 1000	Homogeneous $\sigma_e = 0.0$
1 or 1001	Cylindrical Cell (Sauer's Method) Hex Lattice
2 or 1002	Cylindrical Cell (Sauer's Method) Square Lattice
3 or 1003	Symmetric Slab Cell
4 or 1004	Asymmetric Slab Cell
5 or 1005	Isolated Lump (Dancoff = 0.0)
6 or 1006	Cylindrical Cell (Bell Approximation)
7 or 1007	Symmetric Slab Cell (Bell Approximation)
8 or 1008	Cylindrical Cell (Sauer's Method) Hex Lattice w/clad
9 or 1009	Cylindrical Cell (Sauer's Method) Square Lattice w/clad

Note that when ISSOPT > 1000, the code will use potential scattering values in place of total cross section in determining σ_0 values and will not iterate.

2* Floating-Point Constants [2]
1. EPS – convergence criteria for the Bondarenko iteration (Default = 0.001)
2. A – geometrical escape probability adjustment factor. See notes below on this parameter (Default = 0.0).

T Terminate Data Block 1.

Data Block 2

3$ Mixture numbers in the mixing table [MS]
4$ Component (nuclide) identifiers in the mixing table [MS]
5* Concentrations (atoms/b-cm) in the mixing table [MS]

6$ Mixtures by zone [IZM]
7* Outer radii (cm) by zone [IZM]
8* Temperature (k) by zone [IZM]
9* Extra cross section (cm^{-1}) by zone [IZM]
10$ New identifier for components in the mixing table [MS]
11$ Zone-type identifiers 0 – fuel zone
1 – moderator zone
2 – cladding zone
12* Temperature (K) of the nuclide in a one-to-one correspondence with the mixing table arrays.
T Terminate Data Block 2.

This concludes the input data required by BONAMI.

F1.5.1 NOTES ON INPUT

In the 1$ array, IGR specifies the geometry. This is used in conjunction with the 7* array to calculate the volumes of each zone.

IZM, the number of zones, may or may not mock a real situation. It may, for example, be used to specify IZM independent infinite media when IGR, ISSOPT, and the entries in the 11$ array are properly selected. It can also be used to perform a cell calculation in parallel with one or more infinite medium calculations, if properly directed. In this case, the entries in the 11$ array for the infinite medium zones would be other than 0, 1, or 2.

The value for ISSOPT should be selected from the desired option discussed in Sect. F1.3 of this report.

In the 2* array, EPS is used to specify the convergence expected on all macroscopic total values by zone, that is, each $\Sigma_t(g,j)$ in group g and zone j is converged such that

$$\frac{|\Sigma_t^i(g,j) - \Sigma_t^{i-1}(g,j)|}{\Sigma_t^i(g,j)} \leq \text{EPS} .$$

The "A" factor in the 2* array is the parameter used to adjust the Wigner rational approximation for the escape probability to a more correct value. It has been suggested that if one wishes to use one constant value, A should be 1.0 for slabs and 1.35 otherwise. In the ordinary case, BONAMI defaults A to zero and uses a prescription[8] worked out by Otter to determine a cross-section geometry-dependent value of A which is much more accurate than the single value. The user who wishes the constant value can, however, use it by inputting a value other than zero.

The 3$, 4$, and 5* arrays are used to specify the concentrations of the constituents of all mixtures in the problem as follows:

Entry	3$ (Mixture Number)	4$ (Nuclide ID)	5* (Concentrations)
1			
2			
.			
.			
.			
.			
MS			

The entries in these three arrays are in a one-to-one correspondence among themselves and also with the 10$ and 12* arrays. The 10$ array provides a means of changing the identifier of any nuclide used in the problem. In the event that the number of zones, IZM, is more than one and when an entry in the 10$ array is zero, BONAMI will automatically form a new identifier which is

original ID – 0 – zone number.

For example, a nuclide in zone 5 identified by 1111 would become 111105 on the output master library.

Because of the manner in which BONAMI references the nuclides in a calculation, each nuclide in the problem must have a unique entry in the mixing table. This says that one cannot specify a mixture and subsequently load it into more than one zone, such as can be the case with many modules requiring this type of data.

The 12* array is used to allow varying the temperatures by nuclide within a zone. In the event this array is omitted, the 12* array will default by nuclide to the temperatures of the zone containing the nuclide.

The mixture numbers in each zone are specified in the 6$ array. Mixture numbers are arbitrary and need only match up with those used in the 3$ array.

The radii in the 7* array are referenced to a zero value at the left boundary of the system.

In the event the temperatures in the 8* array are not bounded by temperature values in the Bondarenko tables, BONAMI will select the "bound" closest to the value. For example, a request for 273 K for a nuclide with Bondarenko sets at 300, 900, 2100 K would use the 300 K values.

The extra cross sections in the 9* array allow one extra value to be specified by zone. (This array can normally be ignored.) It is used in the calculation of σ_0 as follows:

$$\sigma_0 = \frac{\sum_{n \neq i} N_n \sigma_t^n + \text{SIGH} + \sigma_{extr}}{N_i}$$

In the event one wishes to select cross sections at a fixed σ_0, a mixture with one nuclide with a number density of unity and

$$\sigma_{extra} = \text{desired } \sigma_0$$

will accomplish the request.

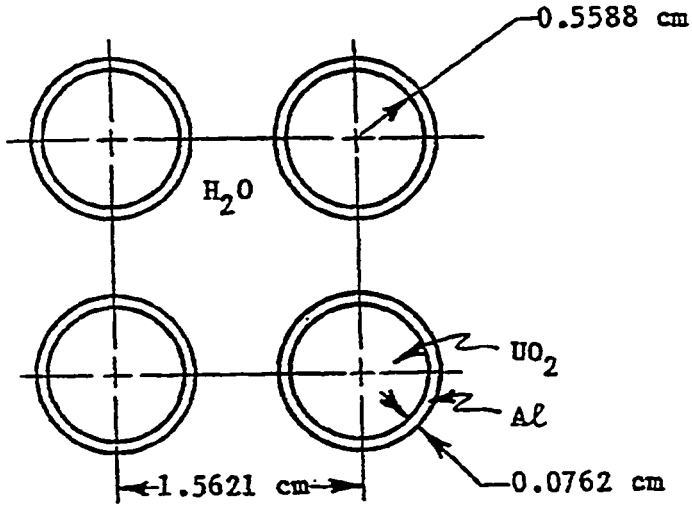
The zone-type identifiers in the 11$ array are used in conjunction with the Dancoff option (ISSOPT) to determine which zones should be combined, etc., in determining a Dancoff factor.

F1.6 SAMPLE PROBLEMS

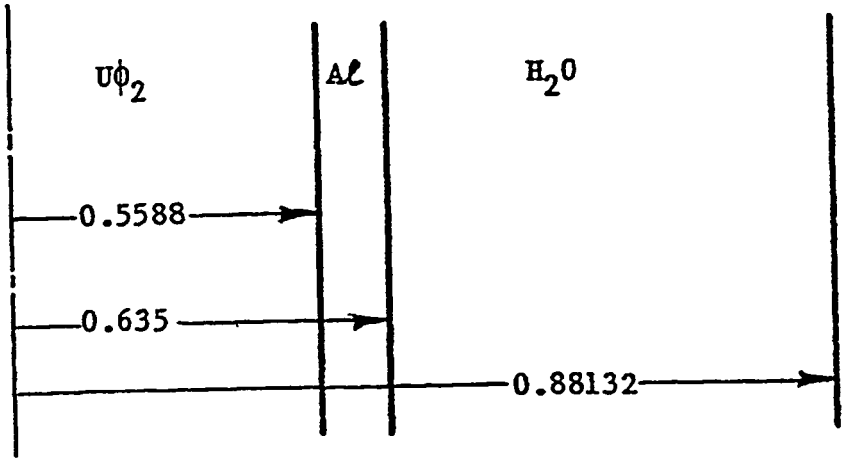
In most cases, the input data to BONAMI are simple and obvious since the complicated parameters are determined internally based on the options selected. The user describes his geometry, the materials contained therein, the temperatures, and a few options.

F1.6.1 SAMPLE PROBLEM 1

This problem is for a system of aluminum-clad UO_2 fuel pins arranged in a square lattice in a water pool.



Following common practice and determining a cylinder whose area is that for the "squares," the following system is to be calculated:



Our number densities are:

UO_2:

$N_{235_U} = 4.881 \times 10^{-4}$

$N_{238_U} = 2.00026 \times 10^{-2}$

$N_O = 4.09815 \times 10^{-2}$

Clad:

$N_{Al} = 6.0245 \times 10^{-2}$

Water:

$N_H = 6.6743 \times 10^{-2}$

$N_O = 3.33371 \times 10^{-2}$

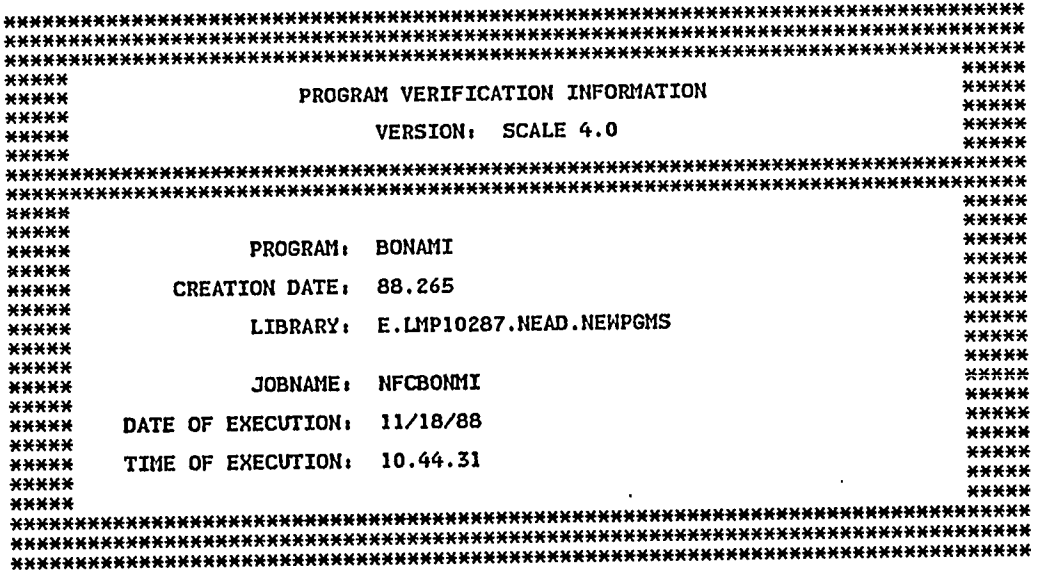
$N^*_{Pb} = 1.0 \times 10^{-2}$

For the problem, we choose ISSOPT = 9 (Sauer's approximation for a cylindrical rod with clad in a square lattice) to account for lattice effects.

A 16-group library is used.

An abbreviated, annotated copy of the output from this case follows:

*Lead is mixed in a trace quantity in order to obtain an infinite dilution set at 300 K.


PROGRAM VERIFICATION INFORMATION
VERSION: SCALE 4.0
PROGRAM: BONAMI
CREATION DATE: 88.265
LIBRARY: E.LMP10287.NEAD.NEWPGMS
JOBNAME: NFCBONMI
DATE OF EXECUTION: 11/18/88
TIME OF EXECUTION: 10.44.31

```
SAMPLE PROBLEM FOR 3 REGION CYLINDRICAL CELL IN SQUARE LATTICE
    0$ ARRAY     4 ENTRIES READ
    1$ ARRAY     6 ENTRIES READ
    0T
```

LOGICAL ASSIGNMENTS

MASTER LIBRARY 3
WORKING LIBRARY 0
SCRATCH FILE 18
NEW LIBRARY 1

P R O B L E M D E S C R I P T I O N

IGR--GEOMETRY (0/1/2/3--INF MED/SLAB/CYL/SPHERE 2

IZM--NUMBER OF ZONES OR MATERIAL REGIONS 3

MS--MIXING TABLE LENGTH 7

IBL--SHIELDED CROSS SECTION EDIT OPTION (0/1--NO/YES) 1

IBR--BONDARENKO FACTOR EDIT OPTION (0/1--NO/YES) 1

ISSOPT--DANCOFF FACTOR OPTION 9

CONVERGENCE CRITERION 1.00000E-03

GEOMETRY CORRECTION FACTOR FOR WIGNER RATIONAL APPROXIMATION 0.000E+00

3$ ARRAY 7 ENTRIES READ

4$ ARRAY 7 ENTRIES READ

5* ARRAY 7 ENTRIES READ

6$ ARRAY 3 ENTRIES READ

7* ARRAY 3 ENTRIES READ

8* ARRAY 3 ENTRIES READ

11$ ARRAY 3 ENTRIES READ

0T

M I X I N G T A B L E

ENTRY	MIXTURE	ISOTOPE	NUMBER DENSITY	NEW IDENTIFIER
1	1	92235	4.88100E-04	9223501
2	1	92238	2.00026E-02	9223801
3	1	8016	4.09815E-02	801601
4	2	13027	6.02450E-02	1302702
5	3	1301	6.67430E-02	130103
6	3	8016	3.33371E-02	801603
7	3	82000	1.00000E-10	8200003

GEOMETRY AND MATERIAL DESCRIPTION

ZONE	MIXTURE	OUTER DIMENSION	TEMPERATURE	EXTRA XS	TYPE (0/1--FUEL/MOD)
1	1	5.58800E-01	3.00000E+02	0.00000E+00	0
2	2	6.35000E-01	3.00000E+02	0.00000E+00	2
3	3	8.81320E-01	3.00000E+02	0.00000E+00	1

THIS CALCULATION REQUIRES 5825 LOCATIONS OF 200000 AVAILABLE TO THIS MODULE

POWER FITTING FOR: 92235-- PROCESSES: 3-- SIGO'S:13-- TEMPERATURES: 1-- MAX GROUPS: 4

POWER FITTING FOR: 92238-- PROCESSES: 2-- SIGO'S:56-- TEMPERATURES: 1-- MAX GROUPS: 5

ZONE	VOLUME	OUTER RADIUS
1	9.810E-01	5.588E-01
2	2.858E-01	6.350E-01
3	1.173E+00	8.813E-01

FUEL REGION VOLUME	9.81E-01
MODERATOR REGION VOLUME	1.17E+00
FUEL REGION RADIUS	5.59E-01
MODERATOR REGION RADIUS	8.81E-01
CLADDING REGION VOLUME	2.86E-01
LBAR IN CLADDING REGION	1.52E-01
WILLIAMS/GILAI CLAD FACTOR	3.09E+00

ELAPSED TIME 0.01 MIN.

INFINITE DILUTION MACROSCOPIC TOTAL CROSS SECTIONS

ZONE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	GROUP 5	GROUP 6	GROUP 7	GROUP 8	GROUP 9	GROUP 10
1	2.413E-01	2.138E-01	3.024E-01	3.137E-01	3.592E-01	4.205E-01	4.847E-01	6.047E-01	1.211E+00	2.355E+00
2	1.389E-01	1.800E-01	1.838E-01	2.316E-01	2.050E-01	9.821E-02	7.732E-02	8.126E-02	8.133E-02	8.148E-02
3	1.910E-01	2.457E-01	3.950E-01	4.904E-01	7.496E-01	1.179E+00	1.422E+00	1.477E+00	1.487E+00	1.490E+00

ZONE	GROUP 11	GROUP 12	GROUP 13	GROUP 14	GROUP 15	GROUP 16
1	1.881E+00	2.705E+00	3.608E-01	3.893E-01	4.743E-01	7.029E-01
2	8.169E-02	8.214E-02	8.279E-02	8.403E-02	8.604E-02	9.424E-02
3	1.491E+00	1.491E+00	1.519E+00	1.606E+00	2.046E+00	3.447E+00

BONDARENKO ITERATION STATISTICS

ITERATION	MT	MAX CHANGE	GROUP	ZONE	NEW VALUE	NUCLIDE	SIGO	FIRST	LAST	TIME(SEC)
1	1	-1.227E-01	11	1	8.317E+01	9223501	5.39362E+03	10	13	3.00E-02
1	1	-8.789E-01	10	1	1.311E+01	9223801	4.85394E+01	8	12	1.00E-02
2	1	-6.621E-02	11	1	7.767E+01	9223501	2.53375E+03	10	13	4.00E-02
2	1	7.796E-03	12	1	2.017E+01	9223801	5.20714E+01	8	12	1.00E-02
3	1	1.049E-04	12	1	7.871E+01	9223501	2.88178E+03	10	13	4.00E-02
3	1	-3.782E-06	12	1	2.017E+01	9223801	5.20689E+01	8	12	1.00E-02
4	ALL GROUPS FOR NUCLIDE		9223801 ARE CONVERGED TO LESS THAN EPS=		1.00E-03					

ELAPSED TIME 0.01 MIN.

SHIELDED MACROSCOPIC TOTAL CROSS SECTIONS

ZONE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	GROUP 5	GROUP 6	GROUP 7	GROUP 8	GROUP 9	GROUP 10
1	2.413E-01	2.138E-01	3.024E-01	3.137E-01	3.592E-01	4.205E-01	4.847E-01	5.794E-01	4.229E-01	4.536E-01
2	1.389E-01	1.800E-01	1.838E-01	2.316E-01	2.050E-01	9.821E-02	7.732E-02	8.126E-02	8.133E-02	8.148E-02
3	1.910E-01	2.457E-01	3.950E-01	4.904E-01	7.496E-01	1.179E+00	1.422E+00	1.477E+00	1.487E+00	1.490E+00

ZONE	GROUP 11	GROUP 12	GROUP 13	GROUP 14	GROUP 15	GROUP 16
1	4.214E-01	5.955E-01	3.608E-01	3.893E-01	4.743E-01	7.029E-01
2	8.169E-02	8.214E-02	8.279E-02	8.403E-02	8.604E-02	9.424E-02
3	1.491E+00	1.491E+00	1.519E+00	1.606E+00	2.046E+00	3.447E+00

NUMBER OF SEPARATE PROCESSES TO TREAT: 5
NUMBER TREATED (INCLUDING MULTI-ZONE): 5
MAXIMUM NUMBER OF SIGMA-0'S: 56
MAXIMUM NUMBER OF TEMPERATURES: 1
OFFSET OF ORIGEN FOR INTERPOLATION: 2.0E+01

MACROSCOPIC ESCAPE CROSS SECTIONS

ZONE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	GROUP 5	GROUP 6	GROUP 7	GROUP 8	GROUP 9	GROUP 10
1	2.410E-01	2.985E-01	4.100E-01	4.813E-01	6.135E-01	7.655E-01	8.339E-01	8.463E-01	8.533E-01	8.534E-01
2	2.135E-01	1.807E-01	2.304E-01	2.348E-01	2.535E-01	2.810E-01	3.126E-01	3.570E-01	2.811E-01	2.969E-01
3	2.135E-01	1.807E-01	2.304E-01	2.348E-01	2.535E-01	2.810E-01	3.126E-01	3.570E-01	2.811E-01	2.969E-01

ZONE	GROUP 11	GROUP 12	GROUP 13	GROUP 14	GROUP 15	GROUP 16
1	8.543E-01	8.495E-01	8.630E-01	8.839E-01	9.716E-01	1.127E+00
2	2.803E-01	3.642E-01	2.473E-01	2.630E-01	3.063E-01	4.044E-01
3	2.803E-01	3.642E-01	2.473E-01	2.630E-01	3.063E-01	4.044E-01

GROUP	FUEL DANCOFF FACTOR	A (GEOMETRY FACTOR)	FUEL TOTAL XS	MODERATOR TOTAL XS	LEFT MODERATOR SIGT
1	7.537E-01	1.532E+00	2.413E-01	2.248E-01	0.000E+00
2	7.011E-01	1.533E+00	2.138E-01	2.896E-01	0.000E+00
3	6.045E-01	1.530E+00	3.024E-01	4.398E-01	0.000E+00
4	5.465E-01	1.529E+00	3.137E-01	5.468E-01	0.000E+00
5	4.455E-01	1.526E+00	3.592E-01	7.995E-01	0.000E+00
6	3.386E-01	1.522E+00	4.205E-01	1.203E+00	0.000E+00
7	2.928E-01	1.517E+00	4.847E-01	1.440E+00	0.000E+00
8	2.831E-01	1.509E+00	5.794E-01	1.497E+00	0.000E+00
9	2.814E-01	1.522E+00	4.229E-01	1.507E+00	0.000E+00
10	2.809E-01	1.520E+00	4.536E-01	1.510E+00	0.000E+00
11	2.808E-01	1.522E+00	4.214E-01	1.511E+00	0.000E+00
12	2.807E-01	1.508E+00	5.955E-01	1.511E+00	0.000E+00
13	2.762E-01	1.526E+00	3.608E-01	1.539E+00	0.000E+00
14	2.627E-01	1.524E+00	3.893E-01	1.626E+00	0.000E+00
15	2.078E-01	1.518E+00	4.743E-01	2.067E+00	0.000E+00
16	1.121E-01	1.498E+00	7.029E-01	3.470E+00	0.000E+00

5825 LOCATIONS OF 5952 AVAILABLE ARE REQUIRED TO MAKE A NEW MASTER CONTAINING THE SELF-SHIELDED VALUES

EDIT FOR MATERIAL: 92235
ZONE: 1
POSITION IN MIX: 1

SHIELDED CROSS SECTIONS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 18 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
10	2.604E+03	6.788E+01	3.788E+01	2.000E+01
11	2.536E+03	7.767E+01	3.921E+01	2.846E+01
12	2.882E+03	7.871E+01	3.115E+01	3.757E+01
13	2.457E+03	4.900E+01	3.000E+01	9.000E+00

EDIT FOR MATERIAL: 92238
ZONE: 1
POSITION IN MIX: 2

SHIELDED CROSS SECTIONS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
8	5.056E+01	1.373E+01	7.340E-01
9	5.131E+01	1.249E+01	1.488E+00
10	5.214E+01	1.320E+01	4.200E+00
11	5.228E+01	1.149E+01	2.494E+00
12	5.207E+01	1.352E+01	4.517E+00

EDIT FOR MATERIAL: 92235
ZONE: 1
POSITION IN MIX: 1

BONDARENKO FACTORS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 18 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
10	2.604E+03	9.983E-01	9.970E-01	1.000E+00
11	2.536E+03	8.727E-01	8.987E-01	8.048E-01
12	2.882E+03	9.371E-01	9.239E-01	9.327E-01
13	2.457E+03	1.000E+00	1.000E+00	1.000E+00

EDIT FOR MATERIAL: 92238
ZONE: 1
POSITION IN MIX: 2

BONDARENKO FACTORS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
8	5.056E+01	9.156E-01	3.670E-01
9	5.131E+01	5.676E-01	1.353E-01
10	5.214E+01	2.237E-01	8.400E-02
11	5.228E+01	1.768E-01	4.453E-02
12	5.207E+01	1.136E-01	4.106E-02

COPY 999 1/V CROSS SECTIO FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 1001 HYDROGEN DE/E FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 1301 HYDROGEN X(E) FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 1002 DEUTERIUM X(E) FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 2004 HELIUM-4 ENDF/B FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 3006 LITHIUM-6 FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 3007 LITHIUM-7 FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 4009 BERYLLIUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 5000 BORON FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 5010 BORON-10 ENDF/B FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 5011 BORON-11 ENDF/B FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 6012 CARBON FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 7014 NITROGEN FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 8016 OXYGEN FROM LOG 3 TO LOG 18 BONDARENKO TRIGGER 0
COPY 8016 OXYGEN FROM LOG 18 TO LOG 1 BONDARENKO TRIGGER 0
COPY 8016 OXYGEN FROM LOG 18 TO LOG 1 BONDARENKO TRIGGER 0
COPY 9019 FLUORINE FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 11023 SODIUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 12000 MAGNESIUM ENDF/ FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 13027 ALUMINUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 14028 SILICON ENDF/B- FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 15031 PHOSPHORUS-31 L FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 16032 SULFUR-32 LENDL FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 17000 CHLORINE FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0

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COPY    19039  POTASSIUM          FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    20040   CALCIUM ENDF/B-   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    22000   TITANIUM ENDF/B   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    23051   VANADIUM ENDF/B   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    24000  CHROMIUM           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    24304   CHROMIUM ENDF/B   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    24404   CHROMIUM ENDF/B   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    25055   MANGANESE-55 EN   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    26000  IRON               FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    26304   IRON ENDF/B-IV    FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    26404   IRON ENDF/B-IV    FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    27059  COBALT             FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    28000  NICKEL             FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    28304   NICKEL ENDF/B-I   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    28404   NICKEL ENDF/B-I   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    29000   COPPER ENDF/B-I   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    30000  ZINC               FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    40000  ZIRCONIUM          FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    40302   ZIRCALLOY-2 END   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    41093  NIOBIUM            FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    42000  MOLYBDENUM         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    47107   SILVER-107 ENDF   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    47109   SILVER-109 ENDF   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    48000   CADMIUM ENDF/B-   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    49113   INDIUM-113 ENDF   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    49115   INDIUM-115 ENDF   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    50000   TIN LENDL MAT 7   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    56138   BARIUM-138 LEND   FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    58000  CERIUM             FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    62000  SAMARIUM           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    63000  EUROPIUM           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
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COPY    64000   GADOLINIUM ENDF FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    66164   DYSPROSIUM-164  FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    71175   LUTETIUM-175 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    71176   LUTETIUM-176 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    72000   HAFNIUM ENDF/B- FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    73181  TANTALUM         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74182   TUNGSTEN-182 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74183   TUNGSTEN-183 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74184   TUNGSTEN-184 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74186   TUNGSTEN-186 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    75185   RHENIUM-185 END FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    75187   RHENIUM-187 END FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    79197   GOLD-197 ENDF/B FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    82000   LEAD ENDF/B-IV  FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    90232  TH-232  INFINITE FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    91233   PROTACTINIUM-23 FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92233  U-233            FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92234   U-234 ENDF/B-IV FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92235  U-235 YR         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 1
COPY    92236   U-236 ENDF/B-IV FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92238  U-238 Y          FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 1
COPY    93237   NP-237 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94238  PU-238           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94338  PU-238 Y         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94239  PU-239           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94240  PU-240           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94241   PU-241 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94242   PU-242 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    95241   AM-241 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    95243   AM-243 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    96244   CM-244 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
```

16 NEUTRON GROUP CRITICALITY SAFETY LIBRARY
BASED ON HANSEN-ROACH DATA WITH SOME ENDF/B VERSION 4 DATA
COMPILED FOR NRC
8/3/81
L.M.PETRIE ORNL

TAPE ID	4321	NUMBER OF NUCLIDES	85
NUMBER OF NEUTRON GROUPS	16	NUMBER OF GAMMA GROUPS	0
FIRST THERMAL GROUP	13	LOGICAL UNIT	1

TABLE OF CONTENTS

1/V CROSS SECTIONS NORMALIZED TO 1.0 AT 0.0253 EV		ID	999
HYDROGEN DE/E	HANSEN ROACH	ID	1001
HYDROGEN X(E)	HANSEN ROACH	ID	130103
DEUTERIUM X(E)	HANSEN ROACH	ID	1002
HELIUM-4 ENDF/B-IV MAT 1270		ID	2004
LITHIUM-6	HANSEN ROACH	ID	3006
LITHIUM-7	HANSEN ROACH	ID	3007
BERYLLIUM	HANSEN ROACH	ID	4009
BORON	HANSEN ROACH	ID	5000
BORON-10 ENDF/B-IV MAT 1273		ID	5010
BORON-11 ENDF/B-IV MAT 1160		ID	5011
CARBON	HANSEN ROACH	ID	6012
NITROGEN	HANSEN ROACH	ID	7014
OXYGEN	HANSEN ROACH	ID	801601
OXYGEN	HANSEN ROACH	ID	801603
FLUORINE	HANSEN ROACH	ID	9019
SODIUM	HANSEN ROACH	ID	11023
MAGNESIUM ENDF/B-IV MAT 1280		ID	12000
ALUMINUM	HANSEN ROACH	ID	1302702
SILICON ENDF/B-IV MAT 1194		ID	14028
PHOSPHORUS-31 LENDL MAT 7019		ID	15031
SULFUR-32 LENDL MAT 7020		ID	16032
CHLORINE	HANSEN ROACH	ID	17000
POTASSIUM	HANSEN ROACH	ID	19039
CALCIUM ENDF/B-IV MAT 1195		ID	20040
TITANIUM ENDF/B-IV MAT 1286		ID	22000
VANADIUM ENDF/B-IV MAT 1196		ID	23051
CHROMIUM	AEROJET	ID	24000
CHROMIUM ENDF/B-IV MAT 1191 SS-304 WT		ID	24304
CHROMIUM ENDF/B-IV MAT 1191 INCONEL WT		ID	24404
MANGANESE-55 ENDF/B-IV MAT 1197		ID	25055
IRON	HANSEN ROACH	ID	26000
IRON ENDF/B-IV MAT 1192 SS-304 WT		ID	26304
IRON ENDF/B-IV MAT 1192 INCONEL WT		ID	26404
COBALT	HANSEN ROACH	ID	27059
NICKEL	HANSEN ROACH	ID	28000
NICKEL ENDF/B-IV MAT 1190 SS-304 WT		ID	28304
NICKEL ENDF/B-IV MAT 1190 INCONEL WT		ID	28404
COPPER ENDF/B-IV MAT 1295		ID	29000
ZINC	GAM-2	ID	30000
ZIRCONIUM	HANSEN ROACH	ID	40000
ZIRCALLOY-2 ENDF/B-IV MAT 1284		ID	40302
NIOBIUM	HANSEN ROACH	ID	41093
MOLYBDENUM	HANSEN ROACH	ID	42000
SILVER-107 ENDF/B-IV MAT 1138		ID	47107
SILVER-109 ENDF/B-IV MAT 1139		ID	47109
CADMIUM ENDF/B-IV MAT 1281		ID	48000
INDIUM-113 ENDF/B-IV MAT 445		ID	49113
INDIUM-115 ENDF/B-IV MAT 449		ID	49115
TIN LENDL MAT 7039		ID	50000
BARIUM-138 LENDL MAT 7040		ID	56138
CERIUM	HANSEN ROACH	ID	58000
SAMARIUM	GAM-2	ID	62000

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                                                                    63000
                                                                    64000
                                                                    66164
                                                                    71175
                                                                    71176
                                                                    72000
                                                                    73181
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                                                                  8200003
                                                                    90232
                                                                    91233
                                                                    92233
                                                                    92234
                                                                  9223501
                                                                    92236
                                                                  9223801
                                                                    93237
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*****************************************************************
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*****************************************************************
*****                                                       *****
*****          PROGRAM VERIFICATION INFORMATION             *****
*****                                                       *****
*****              VERSION:  SCALE 4.0                      *****
*****                                                       *****
*****************************************************************
*****************************************************************
*****************************************************************
*****                                                       *****
*****                                                       *****
*****                                                       *****
*****                PROGRAM:  BONAMI                       *****
*****                                                       *****
*****           CREATION DATE:  88.265                      *****
*****                                                       *****
*****              LIBRARY:  E.LMP10287.NEAD.NEWPGMS        *****
*****                                                       *****
*****                                                       *****
*****                                                       *****
*****               JOBNAME:  NFCBONMI                      *****
*****                                                       *****
*****         DATE OF EXECUTION:  11/18/88                  *****
*****                                                       *****
*****         TIME OF EXECUTION:  10.45.00                  *****
*****                                                       *****
*****                                                       *****
*****************************************************************
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SAMPLE PROBLEM FOR HOMOGENEOUS C:TION
    0$ ARRAY     4 ENTRIES READ
    1$ ARRAY     6 ENTRIES READ
       0T
```

LOGICAL ASSIGNMENTS

MASTER LIBRARY 3
WORKING LIBRARY 0
SCRATCH FILE 18
NEW LIBRARY 1

P R O B L E M D E S C R I P T I O N

IGR--GEOMETRY (0/1/2/3--INF MED/SLAB/CYL/SPHERE 1

IZM--NUMBER OF ZONES OR MATERIAL REGIONS 1

MS--MIXING TABLE LENGTH 6

IBL--SHIELDED CROSS SECTION EDIT OPTION (0/1--NO/YES) 1

IBR--BONDARENKO FACTOR EDIT OPTION (0/1--NO/YES) 1

ISSOPT--DANCOFF FACTOR OPTION 0

CONVERGENCE CRITERION 1.00000E-03

GEOMETRY CORRECTION FACTOR FOR WIGNER RATIONAL APPROXIMATION 0.000E+00

3$ ARRAY 6 ENTRIES READ

4$ ARRAY 6 ENTRIES READ

5* ARRAY 6 ENTRIES READ

6$ ARRAY 1 ENTRIES READ

7* ARRAY 1 ENTRIES READ

8* ARRAY 1 ENTRIES READ

OT

M I X I N G T A B L E

ENTRY	MIXTURE	ISOTOPE	NUMBER DENSITY	NEW IDENTIFIER
1	1	92235	1.96200E-04	9223501
2	1	92238	8.04141E-03	9223801
3	1	8016	3.25059E-02	801601
4	1	13027	7.05570E-03	1302701
5	1	1301	3.20940E-02	130101
6	1	82000	4.81000E-09	8200001

GEOMETRY AND MATERIAL DESCRIPTION

ZONE	MIXTURE	OUTER DIMENSION	TEMPERATURE	EXTRA XS	TYPE (0/1--FUEL/MOD)
1	1	1.00000E+00	3.00000E+02	0.00000E+00	0

THIS CALCULATION REQUIRES 5703 LOCATIONS OF 200000 AVAILABLE TO THIS MODULE

POWER FITTING FOR: 92235-- PROCESSES: 3-- SIGO'S:13-- TEMPERATURES: 1-- MAX GROUPS: 4

POWER FITTING FOR: 92238-- PROCESSES: 2-- SIGO'S:56-- TEMPERATURES: 1-- MAX GROUPS: 5

ZONE	VOLUME	OUTER RADIUS
1	1.000E+00	1.000E+00

FUEL REGION VOLUME	1.00E+00
MODERATOR REGION VOLUME	0.00E+00
FUEL REGION RADIUS	1.00E+00
MODERATOR REGION RADIUS	1.00E+00

ELAPSED TIME 0.01 MIN.

INFINITE DILUTION MACROSCOPIC TOTAL CROSS SECTIONS

ZONE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	GROUP 5	GROUP 6	GROUP 7	GROUP 8	GROUP 9	GROUP 10
1	2.051E-01	2.252E-01	3.331E-01	3.891E-01	5.289E-01	7.476E-01	8.875E-01	9.629E-01	1.211E+00	1.673E+00

ZONE	GROUP 11	GROUP 12	GROUP 13	GROUP 14	GROUP 15	GROUP 16
1	1.483E+00	1.814E+00	8.850E-01	9.385E-01	1.185E+00	1.951E+00

BONDARENKO ITERATION STATISTICS

ITERATION	MT	MAX CHANGE	GROUP	ZONE	NEW VALUE	NUCLIDE	SIGO	FIRST	LAST	TIME(SEC)
1	1	-1.090E-01	11	1	8.447E+01	9223501	7.46151E+03	10	13	3.00E-02
1	1	-8.672E-01	10	1	1.438E+01	9223801	9.97806E+01	8	12	1.00E-02
2	1	-2.901E-02	11	1	8.202E+01	9223501	4.52632E+03	10	13	4.00E-02
2	1	-1.135E-04	11	1	1.243E+01	9223801	1.00006E+02	8	12	1.00E-02
3	1	-1.891E-07	12	1	8.069E+01	9223501	4.91425E+03	10	13	4.00E-02
3	ALL GROUPS FOR NUCLIDE		9223801 ARE CONVERGED TO LESS THAN EPS=		1.00E-03					

ELAPSED TIME 0.01 MIN.

SHIELDED MACROSCOPIC TOTAL CROSS SECTIONS

ZONE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	GROUP 5	GROUP 6	GROUP 7	GROUP 8	GROUP 9	GROUP 10
1	2.051E-01	2.252E-01	3.331E-01	3.891E-01	5.289E-01	7.476E-01	8.875E-01	9.544E-01	9.001E-01	9.180E-01

ZONE	GROUP 11	GROUP 12	GROUP 13	GROUP 14	GROUP 15	GROUP 16
1	9.041E-01	9.800E-01	8.850E-01	9.385E-01	1.185E+00	1.951E+00

NUMBER OF SEPARATE PROCESSES TO TREAT: 5
NUMBER TREATED (INCLUDING MULTI-ZONE): 5
MAXIMUM NUMBER OF SIGMA-0'S: 56
MAXIMUM NUMBER OF TEMPERATURES: 1
OFFSET OF ORIGEN FOR INTERPOLATION: 2.0E+01

MACROSCOPIC ESCAPE CROSS SECTIONS

ZONE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	GROUP 5	GROUP 6	GROUP 7	GROUP 8	GROUP 9	GROUP 10
1	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

ZONE	GROUP 11	GROUP 12	GROUP 13	GROUP 14	GROUP 15	GROUP 16
1	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

5703 LOCATIONS OF 5952 AVAILABLE ARE REQUIRED TO MAKE A NEW MASTER CONTAINING THE SELF-SHIELDED VALUES

EDIT FOR MATERIAL: 92235
ZONE: 1
POSITION IN MIX: 1

SHIELDED CROSS SECTIONS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 18 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
10	4.605E+03	6.800E+01	3.800E+01	2.000E+01
11	4.526E+03	8.202E+01	4.097E+01	3.105E+01
12	4.914E+03	8.069E+01	3.207E+01	3.863E+01
13	4.460E+03	4.900E+01	3.000E+01	9.000E+00

EDIT FOR MATERIAL: 92238
ZONE: 1
POSITION IN MIX: 2

SHIELDED CROSS SECTIONS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
8	9.777E+01	1.394E+01	9.354E-01
9	9.876E+01	1.317E+01	2.171E+00
10	9.978E+01	1.438E+01	5.378E+00
11	1.000E+02	1.243E+01	3.430E+00
12	1.000E+02	1.519E+01	6.194E+00

EDIT FOR MATERIAL: 92235
ZONE: 1
POSITION IN MIX: 1

BONDARENKO FACTORS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 18 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
10	4.605E+03	1.000E+00	1.000E+00	1.000E+00
11	4.526E+03	9.215E-01	9.389E-01	8.780E-01
12	4.914E+03	9.606E-01	9.511E-01	9.590E-01
13	4.460E+03	1.000E+00	1.000E+00	1.000E+00

EDIT FOR MATERIAL: 92238
ZONE: 1
POSITION IN MIX: 2

BONDARENKO FACTORS

GROUP	SIGO	MT= 1 ORDER= 0 OFFSET= 0	MT= 102 ORDER= 0 OFFSET= 0
8	9.777E+01	9.290E-01	4.677E-01
9	9.876E+01	5.987E-01	1.973E-01
10	9.978E+01	2.437E-01	1.076E-01
11	1.000E+02	1.912E-01	6.124E-02
12	1.000E+02	1.277E-01	5.631E-02

COPY 999 1/V CROSS SECTIO FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 1001 HYDROGEN DE/E FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 1301 HYDROGEN X(E) FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 1002 DEUTERIUM X(E) FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 2004 HELIUM-4 ENDF/B FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 3006 LITHIUM-6 FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 3007 LITHIUM-7 FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 4009 BERYLLIUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 5000 BORON FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 5010 BORON-10 ENDF/B FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 5011 BORON-11 ENDF/B FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 6012 CARBON FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 7014 NITROGEN FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 8016 OXYGEN FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 9019 FLUORINE FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 11023 SODIUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 12000 MAGNESIUM ENDF/ FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 13027 ALUMINUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 14028 SILICON ENDF/B- FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 15031 PHOSPHORUS-31 L FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 16032 SULFUR-32 LENDL FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 17000 CHLORINE FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 19039 POTASSIUM FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0
COPY 20040 CALCIUM ENDF/B- FROM LOG 3 TO LOG 1 BONDARENKO TRIGGER 0

```
COPY     22000   TITANIUM ENDF/B FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     23051   VANADIUM ENDF/B FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     24000  CHROMIUM         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     24304   CHROMIUM ENDF/B FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     24404   CHROMIUM ENDF/B FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     25055   MANGANESE-55 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     26000  IRON             FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     26304   IRON ENDF/B-IV  FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     26404   IRON ENDF/B-IV  FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     27059  COBALT           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     28000  NICKEL           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     28304   NICKEL ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     28404   NICKEL ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     29000   COPPER ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     30000  ZINC             FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     40000  ZIRCONIUM        FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     40302   ZIRCALLOY-2 END FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     41093  NIOBIUM          FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     42000  MOLYBDENUM       FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     47107   SILVER-107 ENDF FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     47109   SILVER-109 ENDF FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     48000   CADMIUM ENDF/B- FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     49113   INDIUM-113 ENDF FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     49115   INDIUM-115 ENDF FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     50000   TIN LENDL MAT 7 FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     56138   BARIUM-138 LEND FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     58000  CERIUM           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     62000  SAMARIUM         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     63000  EUROPIUM         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     64000   GADOLINIUM ENDF FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY     66164   DYSPROSIUM-164  FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
```

```
COPY    71175   LUTETIUM-175 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    71176   LUTETIUM-176 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    72000   HAFNIUM ENDF/B- FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    73181  TANTALUM         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74182   TUNGSTEN-182 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74183   TUNGSTEN-183 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74184   TUNGSTEN-184 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    74186   TUNGSTEN-186 EN FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    75185   RHENIUM-185 END FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    75187   RHENIUM-187 END FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    79197   GOLD-197 ENDF/B FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    82000   LEAD ENDF/B-IV  FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    90232  TH-232  INFINITE FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    91233   PROTACTINIUM-23 FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92233  U-233            FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92234   U-234 ENDF/B-IV FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92235  U-235 YR         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 1
COPY    92236   U-236 ENDF/B-IV FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    92238  U-238 Y          FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 1
COPY    93237   NP-237 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94238  PU-238           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94338  PU-238 Y         FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94239  PU-239           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94240  PU-240           FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94241   PU-241 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    94242   PU-242 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    95241   AM-241 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    95243   AM-243 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
COPY    96244   CM-244 ENDF/B-I FROM LOG  3 TO LOG  1    BONDARENKO TRIGGER 0
```

16 NEUTRON GROUP CRITICALITY SAFETY LIBRARY
BASED ON HANSEN-ROACH DATA WITH SOME ENDF/B VERSION 4 DATA
COMPILED FOR NRC
8/3/81
L.M.PETRIE ORNL

TAPE ID	4321	NUMBER OF NUCLIDES	84
NUMBER OF NEUTRON GROUPS	16	NUMBER OF GAMMA GROUPS	0
FIRST THERMAL GROUP	13	LOGICAL UNIT	1

TABLE OF CONTENTS

1/V CROSS SECTIONS NORMALIZED TO 1.0 AT 0.0253 EV		ID 999
HYDROGEN DE/E	HANSEN ROACH	ID 1001
HYDROGEN X(E)	HANSEN ROACH	ID 130101
DEUTERIUM X(E)	HANSEN ROACH	ID 1002
HELIUM-4 ENDF/B-IV MAT 1270		ID 2004
LITHIUM-6	HANSEN ROACH	ID 3006
LITHIUM-7	HANSEN ROACH	ID 3007
BERYLLIUM	HANSEN ROACH	ID 4009
BORON	HANSEN ROACH	ID 5000
BORON-10 ENDF/B-IV MAT 1273		ID 5010
BORON-11 ENDF/B-IV MAT 1160		ID 5011
CARBON	HANSEN ROACH	ID 6012
NITROGEN	HANSEN ROACH	ID 7014
OXYGEN	HANSEN ROACH	ID 801601
FLUORINE	HANSEN ROACH	ID 9019
SODIUM	HANSEN ROACH	ID 11023
MAGNESIUM ENDF/B-IV MAT 1280		ID 12000
ALUMINUM	HANSEN ROACH	ID 1302701
SILICON ENDF/B-IV MAT 1194		ID 14028
PHOSPHORUS-31 LENDL MAT 7019		ID 15031
SULFUR-32 LENDL MAT 7020		ID 16032
CHLORINE	HANSEN ROACH	ID 17000
POTASSIUM	HANSEN ROACH	ID 19039
CALCIUM ENDF/B-IV MAT 1195		ID 20040
TITANIUM ENDF/B-IV MAT 1286		ID 22000
VANADIUM ENDF/B-IV MAT 1196		ID 23051
CHROMIUM	AEROJET	ID 24000
CHROMIUM ENDF/B-IV MAT 1191 SS-304 WT		ID 24304
CHROMIUM ENDF/B-IV MAT 1191 INCONEL WT		ID 24404
MANGANESE-55 ENDF/B-IV MAT 1197		ID 25055
IRON	HANSEN ROACH	ID 26000
IRON ENDF/B-IV MAT 1192 SS-304 WT		ID 26304
IRON ENDF/B-IV MAT 1192 INCONEL WT		ID 26404
COBALT	HANSEN ROACH	ID 27059
NICKEL	HANSEN ROACH	ID 28000
NICKEL ENDF/B-IV MAT 1190 SS-304 WT		ID 28304
NICKEL ENDF/B-IV MAT 1190 INCONEL WT		ID 28404
COPPER ENDF/B-IV MAT 1295		ID 29000
ZINC	GAM-2	ID 30000
ZIRCONIUM	HANSEN ROACH	ID 40000
ZIRCALLOY-2 ENDF/B-IV MAT 1284		ID 40302
NIOBIUM	HANSEN ROACH	ID 41093
MOLYBDENUM	HANSEN ROACH	ID 42000
SILVER-107 ENDF/B-IV MAT 1138		ID 47107
SILVER-109 ENDF/B-IV MAT 1139		ID 47109
CADMIUM ENDF/B-IV MAT 1281		ID 48000
INDIUM-113 ENDF/B-IV MAT 445		ID 49113
INDIUM-115 ENDF/B-IV MAT 449		ID 49115
TIN LENDL MAT 7039		ID 50000
BARIUM-138 LENDL MAT 7040		ID 56138
CERIUM	HANSEN ROACH	ID 58000
SAMARIUM	GAM-2	ID 62000
EUROPIUM	GAM-2	ID 63000

```
GADOLINIUM ENDF/B-IV MAT 1030                                    64000
DYSPROSIUM-164 ENDF/B-IV MAT 1031                                66164
LUTETIUM-175 ENDF/B-IV MAT 1032                                  71175
LUTETIUM-176 ENDF/B-IV MAT 1033                                  71176
HAFNIUM ENDF/B-IV MAT 1034                                       72000
TANTALUM                    HANSEN ROACH                         73181
 TUNGSTEN-182 ENDF/B-IV MAT 1128                                 74182
 TUNGSTEN-183 ENDF/B-IV MAT 1129                                 74183
 TUNGSTEN-184 ENDF/B-IV MAT 1130                                 74184
 TUNGSTEN-186 ENDF/B-IV MAT 1131                                 74186
 RHENIUM-185 ENDF/B-IV MAT 1083                                  75185
 RHENIUM-187 ENDF/B-IV MAT 1084                                  75187
 GOLD-197 ENDF/B-IV MAT 1283                                     79197
 LEAD ENDF/B-IV MAT 1288                                       8200001
TH-232  INFINITE DILUTION        HANSEN ROACH                    90232
  PROTACTINIUM-233 ENDF/B-IV MAT 1297                            91233
U-233                            HANSEN ROACH                    92233
  U-234 ENDF/B-IV MAT 1043                                       92234
U-235 YR                         HANSEN ROACH                  9223501
  U-236 ENDF/B-IV MAT 1163                                       92236
U-238 Y                          HANSEN ROACH                  9223801
  NP-237 ENDF/B-IV MAT 1263                                      93237
PU-238                           HANSEN ROACH                    94238
PU-238 Y                         PERSIMMON                       94338
PU-239                           HANSEN ROACH                    94239
PU-240                           HANSEN ROACH                    94240
  PU-241 ENDF/B-IV MAT 1266                                      94241
  PU-242 ENDF/B-IV MAT 1161                                      94242
  AM-241 ENDF/B-IV MAT 1056                                      95241
  AM-243 ENDF/B-IV MAT 1057                                      95243
  CM-244 ENDF/B-IV MAT 1162                                      96244

   TAPE COPY USED    239 I/O'S, AND TOOK    3.60 SECONDS
```

PRIMARY MODULE ACCESS AND INPUT RECORD (SCALE DRIVER - 11/08/88 - 11.24)

```
*****************************************************************************************************************
*            Messages of current interest to SCALE77 users will appear here                                     *
*                                                                                                               *
*                                        SCALE77                                                                *
*                                                                                                               *
*   ************************************************************************************************            *
*                                                                                                               *
*   11/9/88                                                                                                     *
*     A new equation for the specific gravity of unranyl nitrate solutions has been implemented.  The new       *
*     equation is essentially a reinterpretation of the equation from ARH600.  It fits experimental data        *
*     from Rocky Flats better.  CSAS25, SAS1, and SAS2 have been relinked to make this change.  SAS1 and        *
*     SAS2 have also had minor corrections made.                                                                *
*                                                                                                               *
*    9/08/88                                                                                                    *
*     The expermental SCALE77 procedure has been modified to take advantage of new features and capabilities    *
*     related to VSFortran version 2.2.  Presently CSAS25, SAS2, BONAMI, NITAWL, XSDRN, COUPLE, ORIGEN, and     *
*     KENOVA have been relinked with the new compiler libraries.  Also the SCALE driver has been modified       *
*     so that parameters can be passed to the individual modules from the EXEC line.                            *
*                                                                                                               *
*    9/06/88                                                                                                    *
*     The ORIGEN card image libraries have been updated with revised data.                                      *
*                                                                                                               *
*    7/27/88                                                                                                    *
*     ORIGEN-S has been added to the experimental version of SCALE77, correcting a minor error uncovered        *
*     in the default version.  After testing the default version will be replaced.                              *
*                                                                                                               *
*    6/29/88                                                                                                    *
*     A preliminary version of SAS2 has been added to the experimental version of SCALE77. To access this      *
*     version see below.                                                                                        *
*                                                                                                               *
*    6/3/88                                                                                                     *
*     An experimental version of SCALE77 is now available.  The CSAS4 sequences include the new annular lump    *
*     geometries, and use NITAWL-2 instead of NITAWL. The revised cross section libraries are in the procedure. *
*     To access this version, include the following DD card after your job card.                                *
*                                                                                                               *
*       //PROCLIB DD DSN=LMP.SPF1.PROCLIB,DISP=SHR                                                            *
*                                                                                                               *
*   ************************************************************************************************            *
*                                                                                                               *
* Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning    *
*                                                                                                               *
*    4/25/88                                                                                                    *
*     The default density for Boron in the Standard Composition Library will be changed from 2.535 g/cc to      *
*     2.373 g/cc.  This will bring the density more into line with measurements as well as with the densities   *
*     of B-10 and B-11 in the library.                                                                          *
*                                                                                                               *
* Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning - Warning    *
*                                                                                                               *
*  Further information about these and other updates may be found in NED0.PBF10287.SCALE77.QAFORMS in the member *
*  with the same name as the module.                                                                            *
*                                                                                                               *
*****************************************************************************************************************
```

```
MODULE BONAMI   WILL BE CALLED  TIME OF DAY 10.44.25  DATE 88.323

 ' SAMPLE PROBLEM FOR 3 REGION CYLINDRICAL CELL IN SQUARE LATTICE
 0$$ 3 0 18 1    1$$ 2 3 7 1 1 9 T
 3$$       1          1          1          2          3          3          3
 4$$   92235      92238       8016      13027       1301       8016      82000
 5** 4.881-4 2.00026-2 4.09815-2  6.0245-2  6.6743-2 3.33371-2 1.0-10
 6$$       1          2          3
 7** 0.5588    0.635    0.88132
 8**    300        300        300
 11$$     0          2          1      T
 END

MODULE BONAMI   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED     5.32 (SECONDS). I/O'S USED     805.

MODULE BONAMI   WILL BE CALLED  TIME OF DAY 10.44.54  DATE 88.323

 ' SAMPLE PROBLEM FOR HOMOGENEOUS OPTION
 0$$ 3 0 18 1    1$$ 1 1 6 1 1 0 T
 3$$       1          1          1          1          1          1
 4$$   92235      92238       8016      13027       1301      82000
 5** 1.962-4 8.04141-3 3.25059-2  7.0557-3  3.2094-2    4.81-9
 6$$       1
 7** 1
 8**    300
  T
 END

MODULE BONAMI   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED     5.13 (SECONDS). I/O'S USED     791.
```

F1.7 REFERENCES

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NITAWL-II: SCALE SYSTEM MODULE FOR PERFORMING RESONANCE SHIELDING AND WORKING LIBRARY PRODUCTION

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ABSTRACT

NITAWL-II is a module that must be used with AMPX master cross-section libraries to produce an AMPX working cross-section library that can then be used in a variety of transport calculations, such as those made by XSDRNPM and KENO. The module also provides the Nordheim Integral Treatment for resonance self-shielding. NITAWL-II is used for these purposes in several of the SCALE calculational sequences. This document describes the theory and programming and gives instructions on how to use the program.

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F2.1 INTRODUCTION

The original version of the NITAWL module was developed for the AMPX system.[1] Subsequently, a version of this module called NITAWL-S was developed for the SCALE system and was used exclusively by both SCALE and AMPX until the latter part of 1987, at which time this new version called NITAWL-II was introduced.

All versions of NITAWL perform two major functions. On the basis of a user-specified system description, they perform problem-dependent resonance shielding by applying the Nordheim Integral Treatment.[2] Additionally, NITAWL is used to read cross-section libraries formatted as AMPX master interfaces or as AMPX working interfaces and produce a new library in the AMPX working interface format. The NITAWL module is applied in all SCALE system analytical sequences that involve problem-dependent cross-section processing. NITAWL-II is the new standard used in all these sequences.

The Nordheim method was formulated by L. W. Nordheim in the late 1950s to take advantage of the then-emerging capabilities of second-generation computers in performing rigorous analyses of the energy variation of the neutron flux across resonances. The method was originally programmed by G. F. Kuncir[3] for the IBM-7090 computer. Later versions of Kuncir's programming were incorporated into the GAM-II[4] and XSDRN[5] programs.

Several extensions to the Nordheim calculation have been implemented into the algorithm contained in NITAWL-II.

1. Elements containing more than one isotope can be treated.

2. Self-shielding is applied to resonance scattering. Transfer matrices are adjusted.

3. P-wave as well as s-wave levels can be treated.

4. The asymptotic approximation for the flux in the thermal energy range is assumed to have a Maxwellian energy distribution.

5. A refined procedure for generating the energy mesh over which reaction rates are integrated has been developed.

6. The user has the option of averaging the multigroup constants over the absorber region or with a cell-averaging formulation.

7. New expressions for the absorber region escape probabilities allow the treatment of annular regions.

The AMPX master interface is organized into one-dimensional (1-D) and two-dimensional (2-D) arrays by reaction type, scattering expansion order, and energy groups. Also, resolved resonance data are carried on the interface. (Versions of NITAWL earlier than NITAWL-II also contained provisions for performing an unresolved resonance self-shielding calculation based on techniques taken from the GAM-II code. However, the parameters required by this treatment were such as to preclude its use with any of the unresolved data provided on the ENDF/B libraries issued in the past several versions. Because of this feature and because the BONAMI-S module provides much better unresolved resonance calculational capabilities, it was elected to remove the unresolved resonance techniques from NITAWL-II.) After performing the resonance analysis, NITAWL-II combines the shielded cross sections with the fast and thermal data to produce a working library organized by

reaction type and scattering expansion order. This AMPX working library is compatible with the input requirements of the XSDRNPM, KENO-IV, KENO-V, ICE, MORSE-SGC, and COUPLE modules. The AMPX weighted interface, produced by XSDRNPM, has the same format as the AMPX working interface.

The major difference between NITAWL-S and NITAWL-II is the manner in which it references its self-shielded values to those in the input library. In NITAWL-S, new values were referenced to a set that contained processed values for the resonance wings, for "background" values used to correct deficiencies in parametric fits to experimental data, for p-wave resonances, negative resonances, etc. This procedure required that both the basic data-processing code (primarily the XLACS-II module of AMPX) and NITAWL-S be exactly consistent in the choice of resonance wings and the resonances to be processed. In NITAWL-II, the self-shielding is made with reference to infinite dilution values, a procedure that greatly simplifies the base processing codes, such as XLACS-II, and which allows one to make a Nordheim calculation that can be used with any input library containing the reference infinite dilution values. It also allows one to selectively pick which resonances or kinds of resonances are to be processed, without requiring the basic input library to be regenerated. For example, it could be decided to add processing for p-wave resonances simply by adding the p-wave parameters to the library.

The purpose of this documentation is to describe the current version of NITAWL. Included is a description of the Nordheim Integral Treatment and a discussion of its range of applicability. Also included is a summary of the operations involved in producing working libraries, a description of the program structure in NITAWL-II, and sufficient information for using NITAWL-II as a stand-alone module in SCALE.

F2.2 ANALYTICAL MODEL

F2.2.1 NORDHEIM'S METHOD

The Nordheim Integral Treatment involves a solution for the energy dependence of the neutron flux in a material region containing a resonance absorber and a maximum of two admixed moderators. The material region may be infinite in extent or it may correspond to a 1-D slab, cylinder, or sphere surrounded by a moderating medium in which the neutron flux is spatially flat and varies slowly with energy. The presence of more than one absorber lump in the moderating medium (e.g., a fuel pin lattice) is accounted for through the use of a Dancoff factor.

The collision density as a function of neutron energy, E, is written for this model as

$$\phi(E)\Sigma_T(E) = \sum_{i=1}^{3}\left[((1-P_o^*(E))/\alpha_i)\int_E^{E/(1-\alpha_i)}\phi(E')\Sigma_{si}(E')\frac{dE'}{E'} + P_o^*(E)\,\Sigma_{Ti}(E)W(E)\right], \qquad \text{(F2.2.1)}$$

where

$\phi(E)$ is the neutron flux (neutrons/cm^2-s);

$\Sigma_T(E)$ is the macroscopic total cross section in the absorber (cm^{-1});

i is the nuclide index, i = 1 for the absorber, i = 2 for the first admixed moderator, and i = 3 for the second admixed moderator;

$P_o^*(E)$ is the Dancoff-corrected, first-flight escape probability from the absorber region;

α_i is the maximum fractional energy loss a neutron can suffer in an elastic collision with a nuclide of mass A_i, $\alpha_i = 4A_i/(A_i + 1)^2$ (note that this definition of alpha is 1 minus alpha in many sources);

Σ_{Ti} and Σ_{si} are the macroscopic total and elastic-scattering cross sections of nuclide i, (cm^{-1}); and

W(E) is the assumed energy variation of the neutron flux in the external moderator region. In the epithermal energy range, W(E) is set equal to 1/E. In the thermal energy range, that is, for E < 5 kT, W(E) is set equal to the Maxwellian distribution $CE/(kT)^2 \exp[-E/kT]$, where C is the normalization constant, exp[5]/25, k is the Boltzmann constant, 8.61664×10^{-5} eV/K, and T is the temperature of the medium in Kelvin.

The first term on the right-hand side of Eq. (F2.2.1) is the collision density in the absorber region due to sources arising from isotropic elastic scattering at energies E′ above E. The second term is the collision density due to the flux at the absorber-moderator interface penetrating into the absorber region. The model as defined in Eq. (F2.2.1) involves several approximations.

1. Each resonance nuclide can be treated without consideration of other resonance nuclides which may be present in the system. That is, there is no "resonance overlap" between nuclides taken into account.

2. The neutron flux is spatially uniform in the absorber and moderator regions.

3. Neutron transport into and out of the absorber region can be treated with first-flight escape probabilities.

4. The presence of other absorber lumps in the system can be accounted for with a Dancoff factor. This factor corresponds to the first-flight transmission probability across the moderator. For example, a Dancoff factor of zero corresponds to a single absorber lump isolated by a "sea" of moderator. Conversely, a Dancoff factor of 1.0 corresponds to an infinite medium of absorber material with no external moderator present in the system.

F2.2.2 TWO-REGION RECIPROCITY

The two-region reciprocity theorem of Rothenstein[6] was applied in writing the external moderator source term in Eq. (F2.2.1). Given a two-region system with volumes V_1 and V_2 with isotropic, uniform sources in each region, the first-flight escape probabilities are related by the simple expression

$$P_{01}V_1\Sigma_{T1} = P_{02}V_2\Sigma_{T2} . \qquad \text{(F2.2.2)}$$

If one of the two regions is subdivided into zones (such as multiple fuel rods in a reactor lattice), then the escape probability must include the Dancoff factor discussed above. The second term in Eq. (F2.2.1) is constructed by assuming that the collision rate in the moderator is equal to $V_m\sigma_{TM}W(E)$ and by using Eq. (F2.2.2) to express the escape probability for the moderator in terms of that of the absorber. Cancelling like terms and dividing by the volume of the absorber to obtain the collision density result in the second term in Eq. (F2.2.1). The motivation for this procedure is to eliminate the need for determining the escape probability of the moderator.

Escape probabilities for simple spheres, cylinders, and slabs have been tabulated by Case, deHoffman, and Placzek.[7] Their use represents the spatial transport treatment in the Nordheim method, and thus the geometry is restricted to a relatively simple model. This model is somewhat enhanced in the SCALE system analytical sequences. These sequences obtain the Dancoff factor from algorithms developed for the SUPERDAN program,[8] which includes the effect of cladding material in making its determination. Also, mention should be made of Nordheim's correction of the escape probability for "gray" rods. Since the Dancoff factor is derived for fully absorbing or "black" rods, Nordheim has developed the following formulation to account for the partial transmission through the absorber regions:

$$P_o^*(E) = P_o(E)(1 - C)/\{1 - [1 - \Sigma_T(E)\bar{r}P_o(E)]C\} . \qquad \text{(F2.2.3)}$$

In Eq. (F2.2.3), $P_o(E)$ is the escape probability of Case, deHoffman, and Placzek; C is the Dancoff factor; $\Sigma_T(E)$ is the total cross section of the absorber medium; and $\bar{r}$ is the mean chord length (4 volume/surface) of the absorber region. Equation (F2.2.3) is the expression for the effective escape probability applied in the NITAWL-II program.

The numerical solution of Eq. (F2.2.1) for the collision density and thereby the slowing-down flux spectrum constitutes what is commonly referred to as the Nordheim Integral Treatment. This solution is specified through the selection of option 1 in the 8th, 11th, and 14th entries of the 3* array of the input specifications. Other options available for the absorber for simplifying the solution of the integral terms in Eq. (F2.2.1) are the narrow resonance approximation (option 2) and the infinite mass approximation (option 3).

F2.2.3 NARROW RESONANCE-ASYMPTOTIC FLUX APPROXIMATION

The narrow resonance approximation involves the assumption that the flux, $\phi(E')$, in the source integrals of Eq. (F2.2.1), has the asymptotic form

$$\phi(E') = 1/E' \ . \qquad \text{(F2.2.4)}$$

Equation (F2.2.2) is strictly valid under the following conditions:

1. The moderating medium is infinite in extent, that is, the spectrum is not affected by preferential leakage in some energy range.

2. The moderating medium is nonabsorbing.

3. The energies, E′, are below the source energy range in which spectral oscillations occur over the first few slowing-down intervals, that is, a sufficient number of slowing-down collisions have occurred that $\phi(E')$ has the asymptotic form.

These conditions are generally met in calculating slowing-down sources due to low-absorbing, moderating materials in reactor lattices. The medium is large and low-absorbing. The resonance energy range is well below the source energy range of fission neutrons.

The asymptotic flux approximation also requires that the flux-depletion due to resonance absorption is small relative to the total flux in the slowing-down interval. A criterion for determining the applicability of the narrow resonance approximation involves comparing the practical width of the resonance, Γ_p, with the slowing-down interval, $\alpha E'$. The practical width is given by

$$\Gamma_p = \Gamma(\Sigma_o/(\Sigma_{p1} + \Sigma_{s2} + \Sigma_{s3}))^{\frac{1}{2}} \ , \qquad \text{(F2.2.5)}$$

where Σ_{p1} is the potential scattering cross section of the absorber, and Γ is the width of the resonance measured between the energy points at which the cross section is one-half of its maximum value, Σ_o, corresponding to the resonance base energy, E_o. Thus, if the following condition is met,

$$\Gamma_p << \alpha_1 E_o \ , \qquad \text{(F2.2.6)}$$

then the narrow resonance approximation for the absorber and the asymptotic approximation for the internal moderators may be applied.

Substitution of 1/E′ for $\phi(E')$ and constant scattering cross sections ($\Sigma_{si}(E') = \Sigma_{pi}$) in Eq. (F2.2.1) permit the analytical evaluation of the integral terms. The resulting equation for the collision density is

$$\phi(E)\Sigma_T(E) = \sum_{i=1}^{3} [(1 - P_o^*(E))\Sigma_{pi}/E + P_o^*(E)\Sigma_{Ti}W(E)] . \qquad \text{(F2.2.7)}$$

The numerical evaluation of Eq. (F2.2.7) is much easier than the Nordheim Integral Treatment, Eq. (F2.2.1). The reduced effort involved in solving Eq. (F2.2.7) makes its application preferable for problems in which all of the resonances satisfy the condition given as Eq. (F2.2.6), or the atom density of the absorber is so low ($N < 10^{-5}$ atoms/b-cm) that even a broad resonance would not perturb the flux. This solution is specified through the selection of option 2 in the 8th, 11th, and 14th positions in the 3* array of the input specifications. The solution involves the narrow resonance approximation for the absorber and the asymptotic approximation for the two internal moderators. In the instance that the absorber has resonances with base energies below 5 kT, the asymptotic flux is assumed to be a Maxwellian, and Eq. (F2.2.7) takes the form

$$\phi(E)\Sigma_T(E) = \sum_{i=1}^{3} [(1 - P_o^*(E))\Sigma_{pi} + P_o^*(E)\Sigma_{Ti}]W(E) . \qquad \text{(F2.2.8)}$$

F2.2.4 INFINITE-MASS APPROXIMATION

The infinite-mass approximation pertains to the absorber material. Under this approximation it is noted that the fractional energy loss per collision with the absorber, α_1, approaches zero as the mass of the absorber becomes large. The first term in Eq. (F2.2.1) is evaluated as

$$(1 - P_o^*(E))\phi(E)\Sigma_{s1}(E) \lim_{\alpha_1 \to 0} \int_E^{E/(1-\alpha_1)} \frac{dE'}{\alpha_1 E'} = (1 - P_o^*(E))\phi(E)\Sigma_{s1}(E) . \qquad \text{(F2.2.9)}$$

Substituting Eq. (F2.2.9) into Eq. (F2.2.1) and collecting like terms yields

$$\phi(E) = [\Sigma_T(E) - (1 - P_o^*(E))\Sigma_{s1}(E)]^{-1} \sum_{i=2}^{3} [((1 - P_o^*(E))/\alpha_i) \int_E^{E/(1-\alpha_i)} \phi(E')\Sigma_{si}(E')\frac{dE'}{E'} + P_o^*(E)\Sigma_{Ti}W(E)] . \qquad \text{(F2.2.10)}$$

The qualitative effect of the infinite-mass approximation is to reduce the slowing-down source and, thereby, $\phi(E)$ from the values calculated by the Nordheim Integral Treatment or the narrow resonance approximation. The actual amount of this effect will vary with the relative importance of resonance scattering and resonance absorption, as can be observed from the denominator term of Eq. (F2.2.10). The infinite-mass approximation is selected as option 3 in the 8th position in the 3* array of the input specifications.

F2.2.5 COMPARISON OF MODELS

A comparison of the Nordheim Integral Treatment, the narrow resonance (asymptotic flux) approximation, and the infinite-mass approximation can be drawn from multigroup cross sections processed for a damp bulk-oxide medium and for a light-water-reactor (LWR) fuel pin. The practical widths for the low-energy

resonance of ^{238}U are given in Table F2.2.1. For either of these applications, the narrow resonance criterion, Eq. (F2.2.6), is not satisfied for the lowest four levels. The variation of the processed cross sections given in Tables F2.2.2 and F2.2.3, with the analytical model is virtually the same for both applications. (Note that Tables F2.2.1, F2.2.2, and F2.2.3 were produced by NITAWL-S, the predecessor of NITAWL-II. The results from the two codes have been shown to be equivalent within the accuracies of respective internal procedures, such that the following observations apply to both codes.) Assuming the full Nordheim Integral Treatment (case 1) as the standard, the following observations can be made.

1. The asymptotic flux approximation for the internal moderators is good to within 3%. (Cases 1 and 2)

2. The narrow resonance approximation seriously overestimates the absorption cross section caused by the broad, predominantly absorbing resonance, and it seriously underestimates the absorption cross sections due to the broad resonance with large scattering components. (Cases 1 and 3)

3. The infinite mass approximation is much better than the narrow resonance approximation for these applications. (Cases 1, 3, and 4)

Each of the SCALE system standard analytical sequences (e.g., CSAS4, etc.) specifies resolved resonance processing with the Nordheim Integral Treatment.

F2.2.6 UNRESOLVED RESONANCE TREATMENT

NITAWL-II contains no unresolved resonance treatment. It expects this calculation to be made with the BONAMI-S module of the SCALE system.

F2.2.7 CELL-AVERAGING FORMULATION

The cell-averaging formulation in NITAWL-II is based upon the assumed value, W(E), of the flux in the moderator region. The volume fraction of the absorber region within the lattice cell, VF_a, is entered as the fifteenth parameter in the 3* array. The multigroup cross sections are formulated as

$$\sigma_x^g = VF_a \int_{E_{g-1}}^{E_g} \phi(E')\sigma_x(E')dE' / [VF_a \int_{E_{g-1}}^{E_g} \phi(E')dE' + (1 - VF_a) \int_{E_{g-1}}^{E_g} W(E')dE'] . \quad \text{(F2.2.11)}$$

Since W(E') is generally larger than $\phi(E')$, the result of entering a volume fraction less than unity is to decrease the effective cross sections. This cell-averaging procedure was formulated for use with a special option in XSDRNPM-S in which there is no spatial transport calculated across the lattice cell for the energy groups in the resonance range. A study by Pevey et al.[9] indicates that the procedure is not as accurate as entering a volume fraction of unity and performing the spatial transport over all energy groups. Particularly, the NITAWL-II cell-averaging procedure does not provide a means for cell-averaging constants for nonresonance nuclides such as hydrogen. Therefore, in the SCALE system analytical sequences, the volume fraction in NITAWL-II is set equal to unity and a full transport calculation in XSDRNPM-S is performed.

Table F2.2.1 Low-energy resonances[a] in ^{238}U

Base energy E_o, eV	6.67	20.9	36.8	66.15	80.74
Slowing-down interval $\alpha(^{238}U)\ E_o$, eV	0.111	0.348	0.613	1.102	1.346
Total width Γ, eV	0.0271	0.0356	0.057	0.049	0.026
Peak[b] cross sections total σ_o, b	7513	8469	12209	4493	298
scatter σ_s, b	430	2094	6672	2327	33.4
U_3O_8–H_2O medium practical width Γ_p, eV	0.295	0.413	0.793	0.414	0.057
$\Gamma_p(U_3O_8–H_2O)) << \alpha E_o$	No	No	No	No	Yes
$U(2.8)O_2$ fuel pin practical width Γ_p, eV	0.544	0.759	1.459	0.761	0.104
Γ_p (fuel pin) $<< \alpha E_o$	No	No	No	No	Yes

[a]Resonance data from ENDF/B-IV< MAT No. 1262.
[b]Doppler-broadened to 293 K.

Table F2.2.2 ^{238}U cross sections processed for a damp, bulk-oxide medium[a]

Energy range	3–10 eV		10–30 eV		30–100 eV	
Reaction type	σ_a	σ_s	σ_a	σ_s	σ_a	σ_s
Case 1 ^{238}U: Nordheim H: Nordheim O: Nordheim	6.30 (1.0)	8.94 (1.0)	3.29 (1.0)	9.26 (1.0)	3.37 (1.0)	11.80 (1.0)
Case 2 ^{238}U: Nordheim H: Asymptotic O: Asymptotic	6.49 (1.03)	8.86 (0.99)	3.32 (1.01)	9.20 (0.99)	3.40 (1.01)	11.80 (1.0)
Case 3 ^{238}U: Narrow resonance H: Asymptotic O: Asymptotic	6.79 (1.08)	8.76 (0.98)	3.02 (0.92)	8.89 (0.96)	2.61 (0.77)	10.59 (0.89)
Case 4 ^{238}U: Infinite mass H: Asymptotic O: Asymptotic	6.40 (1.02)	8.85 (0.99)	3.15 (0.96)	9.19 (0.99)	3.23 (0.96)	12.10 (1.03)

[a]$N(^{238}U) = 0.0110$ atoms/b-cm; $N(H) = 0.0209$ atoms/b-cm, $N(O) = 0.0406$ atoms/b-cm; $U_3O_8/H_2O = 2.19$; $H/U = 1.9$.

Table F2.2.3. ^{238}U cross sections processed for a LWR fuel pin[a]

Energy range	3–10 eV		10–30 eV		30–100 eV	
Reaction type	σ_a	σ_s	σ_a	σ_s	σ_a	σ_s
Case 1	6.19	8.86	3.20	9.19	3.28	11.73
^{238}U: Nordheim	(1.0)[b]	(1.0)	(1.0)	(1.0)	(1.0)	(1.0)
O: Nordheim						
Case 2	6.33	8.86	3.23	9.17	3.30	11.72
^{238}U: Nordheim	(1.02)	(1.0)	(1.01)	(0.99)	(1.01)	(1.0)
O: Asymptotic						
Case 3	6.63	8.75	2.95	8.87	2.55	10.55
^{238}U: Narrow resonance	(1.07)	(0.99)	(0.92)	(0.97)	(0.78)	(0.90)
O: Asymptotic						
Case 4	6.23	8.83	3.05	9.15	3.11	11.92
^{238}U: Infinite mass	(1.01)	(0.99)	(0.95)	(0.99)	(0.95)	(1.02)
O: Asymptotic						

[a]$U(2.8)O_2$ at 93% theoretical density, Westinghouse 17 × 17 PWR, Pitch = 1.43 cm, Fuel OD = 0.9294 cm, Clad OD = 1.0719 cm, Gap OD = 1.0528 cm, N(^{238}U) = 0.022 atoms/b-cm, N(O) = 0.044 atoms/b-cm, N(^{235}U) = 0.00059 atoms/b-cm. Dancoff = 0.2345.

[b]The numbers in parentheses are ratios to the Case 1 values.

F2.2.8 RANGE OF APPLICABILITY

Within the scope of the analytical model, the Nordheim Integral Treatment is a rigorous method for processing resonance cross sections. Other methods that treat the same analytical model through various approximations (such as the narrow resonance approximation) are generally more efficient but less accurate. The major limitations of the analytical model are from the following:

1. the treatment of a single resonance absorber located in a single material region;

2. the treatment of external moderation through the assumption of an asymptotic flux present at the absorber-moderator interface; and

3. the treatment of spatial transport with the first-flight escape probability for the absorber, the two-region reciprocity theorem and Dancoff factors.

In general, these are not severe limitations for the analysis of LWR fuel pin cells or for many of the other applications commonly encountered in neutronics analyses. However, in applications involving several isotopes

with large resonances or complicated absorber-moderator geometries, caution should be exercised in using NITAWL-processed cross sections. The presence of more than one resonance isotope in a material can lead to an effect called resonance overlap. It results in either enhanced or reduced group-averaged cross sections, depending upon the predominance of resonance scattering or absorption and the relative locations of the resonances within the energy groups. The resonance overlap effect is discussed in some detail in Sect. M7.A.7.

The restriction of the resonance absorber to a single material region limits the use of the NITAWL program for certain applications. For example, the analysis of machinery for dissolving spent fuel elements may require the simultaneous consideration of the resonance absorbers being located in the solid fuel pellets and in the acid solution. Procedures for treating complicated geometries, as well as resonance overlap, have been developed for the ROLAIDS program described in Ref. 10. The user may find it worthwhile to obtain reference analyses with the ROLAIDS program for systems that do not match the analytical model.

The low-order transport model where elastic scattering is treated as isotropic in the laboratory system is generally considered to be adequate for most applications. However, there are instances in which the isotropic and uniform sources assumed in deriving the escape probabilities and Dancoff factors do not hold. The importance of treating anisotropic scattering and flux components can be determined through the use of the XSDRNPM-S module.

In addition to the effect upon the cell-averaged constants discussed in Sect. F2.2.7, the assumption of an asymptotic flux in the moderator region does not provide for the treatment of thermal upscatter in the presence of the large thermal resonances. As discussed in Sect. M4.1, the overall approach taken in developing the SCALE system cross-section libraries has been to assume a Maxwellian-shaped thermal moderator flux in performing the resonance processing and also to include enough thermal energy groups so that the gross effects of thermal upscatter are treated in the subsequent Monte Carlo or discrete-ordinates transport analyses. This procedure also accommodates the treatment of those thermal resonances that are described with point cross sections rather than resonance parameters in the ENDF/B specifications.

Finally, another aspect of the Nordheim Integral Treatment that occasionally limits its use arises not from the analytical model, but from the procedure of treating each resonance independently in obtaining the numerical solution. Two effects due to this procedure have been identified:

1. In analyzing the large s-wave levels in ^{238}U metal systems, it was found that the scattering cross sections in the wings of the resonances were up to 15% too small due to the neglect of contributions from the higher-energy resonances. These approximate results cause too much flux depletion in the resonance wings and overall high values for the group-averaged constants.

2. In analyzing the relatively narrow and predominantly scattering resonances of zirconium in the intermediate energy range, it was found that the presence of several significant resonances in a single energy group coupled with the independent averaging of each resonance leads to inconsistent values for the group-averaged constants. This effect, which usually is not noticeable, arises from the assumption of a "fresh" asymptotic slowing-down flux at an energy, E, above each resonance. This assumption precludes the possibility of accumulating the flux-averaging integrals in Eq. (F2.2.15) in a fully consistent manner.

Many years of experience with the Nordheim Integral Treatment as applied in NITAWL-II have yielded the following general estimates of the accuracy of the method for various applications:

1. In the analysis of LWR fuel pin cells, the method yields group-averaged constants that agree with those produced by more rigorous methods (ROLAIDS, Monte Carlo) to within 5%. Reactivity biases of up to 0.5% $\Delta k/k$ have been observed.

2. For the more unusual applications that do not match the analytical model, errors in group-averaged constants of 30% and reactivity biases as high as 3% have been observed. Note that in the case of the zirconium-scattering resonances described above, the numerical procedure essentially "breaks down" and much larger effects are observed.

These levels of accuracy should be considered in the context of order-of-magnitude errors in group-averaged constants and reactivity biases as high as 30%, resulting from the application of nonshielded cross-section data. From this viewpoint, the Nordheim Integral Treatment is seen to be very satisfactory for most important applications and less accurate but still useful for analyzing the more unusual systems.

F2.3 NUMERICAL PROCEDURES

F2.3.1 OUTLINE OF PROCEDURE

The numerical solutions of Eqs. (F2.2.1), (F2.2.7), and (F2.2.10) for the collision density in the resolved resonance energy range and subsequent cross-section averaging are performed in the following sequence:

1. The equations for the collision density are converted from the energy variable into the lethargy variable, $u = \ell n(E_1/E)$. The macroscopic cross sections are divided by the atom density of the absorber. This mechanism normalizes the collision density to one absorber atom.

2. Each resonance is treated separately. This separation allows the determination of an energy E_1 above each resonance at which an asymptotic slowing-down flux can be assumed. Based upon the slowing-down interval of the absorber, an integration mesh is defined for each resonance. The scattering cross sections of the internal moderators are adjusted to produce the correct slowing-down sources when integrated over this mesh.

3. Starting with the asymptotic source from above each resonance, a backward integration by Simpson's rule summation is performed to obtain the variation of the collision density across the resonance. The number (1, 2, or 3) of running integrations performed will depend on the model selections for the absorber and internal moderator contributions to the slowing-down source.

4. At each lethargy interval, point values of the resonance cross sections and a first-flight escape probability for the absorber are calculated for use in determining the collision density.

5. After the collision density across each resonance is determined, the associated flux distribution is used to weight the reaction cross sections over the desired broad group structure. The cell-averaging option described in Sect. F2.2.7 is performed at this point.

The numerical procedures involved in each of the steps 1 through 6 are described briefly.

F2.3.2 SLOWING-DOWN EQUATIONS IN THE LETHARGY VARIABLE

In converting the equations for the collision density to the lethargy variable, the following relationships are applied:

$$F(E) \equiv \phi(E)\,\Sigma_T(E) \qquad \text{(F2.3.1)}$$

$$u \equiv \ell n(E_1/E) \rightarrow du = -\,dE/E\ . \qquad \text{(F2.3.2)}$$

With the definitions (F2.3.1) and (F2.3.2), the integrands in the slowing-down source terms become

$$\phi(E)\Sigma_{si}(E)dE/E = -\,F(u)\Sigma_{si}(u)du/\Sigma_T(u)\ . \qquad \text{(F2.3.3)}$$

The integration ranges corresponding to the slowing-down intervals become

$$\Delta u_i = \ell n[E_1/E] - \ell n[E_1(1 - \alpha_i)/E] = \ell n[1/(1 - \alpha_i)] \ . \qquad \text{(F2.3.4)}$$

The lethargy and energy variables range in opposite directions. Reversing the integration limits/cancels the minus sign in the new expression for the integrands, Eq. (F2.3.3).

The reaction rates are normalized to one absorber atom. Division by the number density of the absorber, N_1, results in the following definitions for effective cross sections:

$$\sigma_T(u) = \Sigma_T(u)/N_1 \ , \qquad \text{(F2.3.5)}$$

$$\sigma_{Ti}(u) = \Sigma_{Ti}(u)/N_1 \ , \qquad \text{(F2.3.6)}$$

$$\sigma_{si}(u) = \Sigma_{si}(u)/N_1 \ . \qquad \text{(F2.3.7)}$$

$$\sigma_{pi} = \Sigma_{pi}/N_1 \ . \qquad \text{(F2.3.8)}$$

Applying the above relationships collectively to Eq. (F2.2.1) for the Nordheim Integral Treatment yields:

$$F(u) = \sum_{i=1}^{3} [((1 - P_o^*(u))/\alpha_i) \int_{u-\Delta u_i}^{u} F(u')(\sigma_{si}(u')/\sigma_T(u'))du' + P_o^*(u)\, \sigma_{Ti}(u)W(u)], \qquad \text{(F2.3.9)}$$

where

$$W(u) = e^u/E_1 \ , E \geq 5\ kt \ ,$$

or

$$W(u) = (5.936526\ /(kT)^2)E_1\, e^{-u} e^{\left(-\frac{E_1 e^{-u}}{kT}\right)} \ , E < 5\ kT \ .$$

Similarly, Eq. (F2.2.7) for the narrow resonance-asymptotic flux approximation becomes

$$F(u) = \sum_{i=1}^{3} (1 - P_o^*(u))\, \sigma_{pi} + P_o^*\, \sigma_{Ti}(u)W(u) \ , \qquad \text{(F2.3.10)}$$

and Eq. (F2.2.10) for the infinite-mass approximation becomes

$$F(u) = [1 - (1 - P_o^*(u))\sigma_{s1}(u)/\sigma_T(u)]^{-1} \sum_{i=2}^{3} [((1 - P_o^*(u))/\alpha_i) F(u') (\sigma_{si}(u')/\sigma_T(u'))du' + P_o^*(u)\sigma_{Ti}(u)W(u)] . \quad \text{(F2.3.11)}$$

F2.3.3 DETERMINATION OF E_1, INTEGRATION MESH INTERVAL, AND SLOWING-DOWN POWER CONSERVATION

This algorithm differs from the one originally programmed by Kuncir[3] in two respects:

1. An integration mesh is determined for each resonance that contains a specified number of points (501 by default). Note that NITAWL-S used an iterative procedure that determined a variable number of points for each resonance.

2. The average lethargy gain per collision, xi_i, rather than the maximum fractional energy loss per collision, α_i, is applied in adjusting the internal moderator cross sections to conserve their slowing-down powers.

With the exception of the cross-section adjustment, these functions are performed in subroutine GRID.

The initial estimate for the energy, E_1, above the resonance base energy, E_0, at which to start the slowing-down calculation is based upon taking the maximum of a factor s/2 times the practical width, Γ_p, or 10 times the Doppler width, Γ_D.

$$E_1 = E_0 + X\Gamma , \quad \text{(F2.3.12)}$$

where

$$X = MAX \left| \frac{s}{2}\Gamma_p, 10\Gamma_D \right| ;$$

$$\Gamma_p = \Gamma\sqrt{\sigma_0/\sigma_{P1}}, \ \sigma_0 = 2.6 \times 10^6 \, g\Gamma_n/(E_0\Gamma) ;$$

and

$$\Gamma_D = \sqrt{4E \, kT/A} .$$

Experience has shown that the factor X in Eq. (F2.3.12) is sometimes too large. Prior to the determination of E_1, it is compared to another factor Y, whose determination is described below, after which it is taken to be in minimum of the above value and Y; that is,

$$X = MIN \left| X, Y \right| . \quad \text{(F2.3.13)}$$

Define a parameter d by

$$d = 2\,\ell n\left(\frac{A+1}{A-1}\right), \qquad \text{(F2.3.14)}$$

which is closely related to the log of the parameter α_i in Eq. (F2.2.1). Then define Δ_o by

$$\Delta_o = e^{(MESH-1)d}, \qquad \text{(F2.3.15)}$$

where MESH is the number of points to be assigned to each resonance. The parameter Δ_o is the lethargy span that could be attained if a neutron scattered elastically (MESH–1) times, losing the maximum energy at each collision. Now define Y as

$$Y = \frac{\Delta_o - 1}{\Delta_o + 1}\,\frac{E_o}{\Gamma}. \qquad \text{(F2.3.16)}$$

In the event that Y is less than X, it replaces X as in Eq. (F2.3.13) and is used to determine E_1 as in Eq. (F2.3.12). The bottom energy, E_2, for the resonance is then determined from

$$E_2 = E_0 - X\Gamma. \qquad \text{(F2.3.17)}$$

Unfortunately, this simple procedure does not always give an adequate range of coverage, especially for resonances at low energies. An iterative procedure, therefore, is used which is similar to one in the original GAM-II coding, but it has been modified to cover specific situations more effectively. Because this procedure did not derive from an orderly development, it is difficult to describe in a supported manner. The following will document the procedure, but will make no attempt to explain why the particular selection of parameters was made.

Define a parameter, r, by

$$r = (5 + \frac{1}{2}\sqrt{kTE_0/A})/\Gamma,$$

and set an initial guess at the lethargy spacing for a mesh over the resonance to

$$\epsilon = 2/\left[A\ \text{Integer}\left(\frac{r}{2}\sqrt{\frac{E_0}{AkT}} + 1\right)\right]. \qquad \text{(F2.3.18)}$$

The iteration starts by looking at a parameter, Z_1, defined by

$$Z_1 = (E_1 - E_0)/E_0.$$

When $Z_1 \le \frac{4}{7}$, set

$$M = 1 + 2\,\text{Integer}\left[\ell n \frac{E_1}{2E_0 - E_1}/2\epsilon + 1\right],$$

$$U_2 = e^{M\epsilon},$$

$$E_1 = 2E_0/(1 + e^{-U_2}).$$

Otherwise, set

$$M = 1 + 2\,\text{Integer}\left[\ell n \frac{7E_1}{3E_0}/2\epsilon + 1\right],$$

$$U_2 = e^{M\epsilon},$$

$$E_1 = 3\,E_0\ e^{-U_2}/7\ .$$

An input parameter, MMSH, specifies the number of mesh intervals to be taken with each resonance. (It is set to 500 by default). If the ratio, q = M/MMSH, is greater than 0.9, the iteration is satisfied and the code proceeds to calculate parameters associated with the resonance energy mesh, as described below. Otherwise, the parameter, ϵ, is recalculated by

$$\epsilon' = 2q\epsilon/(1 + \epsilon),$$

where ϵ' will then replace ϵ.

Then $U_2 = e^{MMSH\cdot\epsilon}$.

If $U_2 > \frac{11}{3}$,

$E_1 = 3U_2\,E_0/7$.

Otherwise,

$E_1 = 2\,E_0\,U_2/(1 + U_2)$,

and the code returns to the point where the parameter Z_1 was calculated and repeats the sequence just described.

When the iteration is satisfied, the number of intervals to use for the resonance is set to MMSH, after which it calculates

$$N = 2\left[\frac{\text{Integer}\left(\frac{d}{\epsilon}\right) + 1}{2}\right], \qquad \text{(F2.3.19)}$$

$$\epsilon = \frac{d}{N},$$

$$U_2 = e^{MMSH\cdot\epsilon},$$

$$E_1 = 2E_0U_2/(1+U_2). \qquad \text{(F2.3.20)}$$

The three parameters, ϵ, MMSH, and E_1, are those parameters that it will use later to construct the mesh for the resonance.

With the integration mesh determined, the next step is to establish the number of integration intervals required to cover the integration ranges given in Eq. (F2.3.4). Making use of the relations

$$\ell n[1/(1-\alpha_i)] \simeq \alpha_i \simeq 4/A_i \ (\alpha_i \text{ small}), \qquad \text{(F2.3.21)}$$

the number of intervals for integrating the slowing-down density due to the absorber is given by

$$n_1 = [1.5 + 4/(A_1\,\epsilon)]. \qquad \text{(F2.3.22)}$$

The bracket denotes truncation to the nearest integer. Recall that Eq. (F2.3.19) for ϵ was developed such that n would be an even integer. Similar expressions must be obtained for the number of intervals used in integrating the internal moderator terms. These expressions are

$$n_i = 1 + 2*\text{INTEGER}\,[\ell n(1/(1-\alpha_i))/2\epsilon + 1];\ i = 2,3. \qquad \text{(F2.3.23)}$$

Now, since ϵ was determined on the basis of α_i, the fractional energy loss due to a collision with the absorber, there is little likelihood that even numbers of mesh intervals will fit exactly fit the integration ranges for the moderators. Therefore, using Eq. (F2.3.23), the α_i are redefined as

$$\alpha_i^* = 1 - e^{-\epsilon n_i},\ i = 2,3. \qquad \text{(F2.3.24)}$$

Also, the moderator cross sections are adjusted to conserve the slowing-down power by the prescription

$$\sigma_{si}^* = \sigma_{si}\,\xi_i/\xi_i^*,\ i = 2,3, \qquad \text{(F2.3.25)}$$

where

$$\xi_i = 1 + [(1-\alpha_i)/\alpha_i]\ell n(1-\alpha_i)$$

and

$$\xi_i^* = 1 + [(1 - \alpha_i^*/\alpha_i^*]\ell n(1 - \alpha_i^*) .$$

For an infinite medium of pure scatterers, the lethargy-dependent slowing-down density, q(u), is equal to the slowing-down power, $\xi\sigma_s$, times the lethargy-dependent flux, $\phi(u)$. Thus, the slowing-down sources due to the internal moderators are conserved under this procedure.

F2.3.4 NUMERICAL INTEGRATION WITH SIMPSON'S RULE

The collision densities, as given by the various models, Eqs. (F2.3.9), (F2.3.10), and (F2.3.11), are combined into a single expression with a "switch" on each term set by the user-specified input.

$\delta(N_1)$ - Nordheim Integral Treatment for the Absorber
$\delta(N_2)$ - Nordheim Integral Treatment for the First Moderator
$\delta(N_3)$ - Nordheim Integral Treatment for the Second Moderator
$\delta(NR)$ - Narrow Resonance Approximation for the Absorber
$\delta(A_1)$ - Asymptotic Flux Approximation for the First Moderator
$\delta(A_2)$ - Asymptotic Flux Approximation for the Second Moderator
$\delta(IM)$ - Infinite Mass Approximation for the Absorber
$\delta(EM)$ - Heterogeneous System with External Moderator

Incorporating these switches and the above definitions for the adjusted cross sections, this single expression for the collision density becomes

$$\begin{aligned} F(u) = (1 - P_o^*(u))[&\delta(N_1)/\alpha_1 \int_{u-n_1\epsilon}^{u} F(u')\sigma_{s1}(u')/\sigma_t(u')du' \\ &+ \delta(N_2)/\alpha_2^* \int_{u-n_2\epsilon}^{u} F(u')\sigma_{s2}^*/\sigma_t(u')du' \\ &+ \delta(N_3)/\alpha_3^* \int_{u-n_3\epsilon}^{u} F(u')\sigma_{s3}^*/\sigma_t(u')du' \\ &+ (\delta(NR)\sigma_{p1} + \delta(A_1)\sigma_{s2} + \delta(A_2)\sigma_{s3})W(u) \\ &+ \delta(IM)F(u)\sigma_{s1}(u)/\sigma_t(u)] + \delta(EM)P_o^*(u)\sigma_t(u)W(u) , \end{aligned} \qquad \text{(F2.3.26)}$$

where

$$\sigma_t(u) = \sigma_{t1}(u) + \delta(N_2)\sigma_{s2}^* + \delta(N_3)\sigma_{s3}^* + \delta(A_1)\sigma_{s2} + \delta(A_2)\sigma_{s3} .$$

Evaluation of the integral terms in Eq. (F2.3.26) by Simpson's rule yields an end-point contribution and an incomplete integral of the form:

$$1/\sigma \int_{u-n\epsilon}^{u} F(u')\sigma_s(u')/\sigma_t(u')du' = \epsilon/(3\alpha)[F(u)\sigma_s(u)/\sigma_t(u) + \overset{u-\epsilon}{\underset{u-n\epsilon}{I}} F(u')\sigma_s(u')/\sigma_t(u')] , \quad \text{(F2.3.27)}$$

where the incomplete integral consists of

$$\overset{u-\epsilon}{\underset{u-n\epsilon}{I}} F(u')\sigma_s(u')/\sigma_t(u') = 2\sum_{i=1}^{2}(3-i)\sum_{j=1}^{n/2-i+1} F(u-k\epsilon)\sigma_s(u-k\epsilon)/\sigma_t(u-k\epsilon)$$

$$+ F(u-n\epsilon)\sigma_s(u-n\epsilon)/\sigma_t(u-n\epsilon) ,$$

with the integer $k = 2j + i - 2$.

Now, applying Simpson's rule to the integrals in Eq. (F2.3.28) and collecting terms on the collision density results in

$$\begin{aligned} F(u) = \{1 - 11(1 - P_o^*(u))[\epsilon/(3\sigma_t(u))\delta(N_1)\sigma_{s1}(u)/\alpha_1 + \delta(N_2)\sigma_{s2}^*/\alpha_2^* + \delta(N_3)\sigma_{s3}^*/\alpha_3^* \\ + \delta(IM)\sigma_{s1}(u)/\sigma_t(u)]\}^{-1} \times \{(1 - P_o^*(u))[\delta(N_1)/\alpha_1 \overset{u-\epsilon}{\underset{u-n\epsilon}{I}} F(u')\sigma_{s1}(u')/\sigma_t(u') \\ + \delta(N_2)/\alpha_2^* \overset{u-\epsilon}{\underset{u-n\epsilon}{I}} F(u')\sigma_{s2}^*/\sigma_t(u') + \delta(N_3)/\alpha_3^* \overset{u-\epsilon}{\underset{u-n\epsilon}{I}} F(u')\sigma_{s3}^*/\sigma_t(u')] \\ + [(1 - P_o^*(u))(\delta(NR)\sigma_{P1} + \delta(A_1)\sigma_{s2} + \delta(A_2)\sigma_{s3}) \\ + \delta(EM)P_o^*(u)\sigma_t(u)]W(u)\} . \end{aligned} \quad \text{(F2.3.29a)}$$

The incomplete integrals are evaluated in subroutine SIMPSN. Tables are constructed to represent the distinct integrands within each integration interval. The initial values in these tables are the back integrands corresponding to the integration of sources due to the asymptotic flux above E_1 or below $u = 0$. That is, these sources are

$$F(E) = 1/\alpha \int_{E_1}^{E_1/(1-\alpha)} \sigma_s dE'/(E')^2 = F(u) = -\sigma_s/(\alpha E_1)\int_0^{u-\Delta u} e^{u} du' . \quad \text{(F2.3.29b)}$$

Therefore, the integrand evaluated over the first interval of width $-\epsilon$ is

$$BVAL(1) = \sigma_s e^{-\epsilon}/(\alpha E_1) ; \quad \text{(F2.3.29c)}$$

the integrand evaluated at the last interval is

$$BVAL(m) = \sigma_s e^{-m\epsilon}/(\alpha E_1) . \quad \text{(F2.3.30)}$$

Note that $m\epsilon = \Delta u$, the total slowing-down interval of Eq. (F2.3.4).

Taking advantage of the constant integration interval size, a running value of the Simpson's rule summation [cf. Eq. (F2.3.27)] for each incomplete integral is stored at each lethargy u after the addition of the

$(u-\epsilon)^{th}$ term and subtraction of the $(u-m\epsilon)^{th}$ term. This procedure avoids the recalculation of the major portion of the slowing-down source at each lethargy. Thus, it results in a very efficient technique for the numerical evaluation of the slowing-down source integrals. The procedure is completed by moving over the integration mesh in the positive lethargy range and determining the integrand values numerically as $F(u)\sigma_s(u)/\sigma_t(u)$ for use in subsequently evaluating the collision density $F(u+\epsilon)$.

F2.3.5 GROUP-AVERAGING PROCEDURES

NITAWL-II contains no provisions for wing treatments as in previous versions of the code, nor does it require that the basic processing code used to produce multigroup libraries preprocess the wings into, for example, background cross sections. It is formulated in such a manner to allow one to use the Nordheim treatment with a library that contains infinite-dilution-weighted cross sections. This result is accomplished by formulating the resonance processing such that it determines the difference between self-shielded values and the corresponding infinite dilution values, instead of just calculating self-shielded values that either replace or add to preprocessed background values.

This new formulation has several advantages over any of the previous implementations:

1. It makes the preprocessing code simpler by removing any requirement that it have prior knowledge of the Nordheim treatment; for example, it does not have to produce background cross sections that contain "wings," $\ell = 1$ resonances, etc.

2. Since the output of the calculation is a difference between the shielded value and an infinite dilution value, the effect of using different procedures (integration schemes, energy meshes, etc.) is a second-order error.

3. The new treatment allows one to decide which resonances or group of resonances ($\ell = 0$, $\ell = 1$, etc.) are important enough to include in the treatment.

All this is accomplished by making the Nordheim treatment determine point cross-section values at two temperatures: (1) the "problem" temperature, and (2) a reference temperature at which the basic cross sections were produced. The reference temperature is carried as part of the resonance information on the master cross-section library. After the cross sections are determined, the flux calculation is made, exactly as in previous versions of NITAWL, using the cross sections at the problem temperature. Both sets of cross sections are then passed to TRAPZ, the subroutine in which the point values are group averaged. The point values at the problem temperature are averaged over the problem fluxes, while the values at the "reference" temperature are averaged using a smooth function, consisting of a 1/E flux tied to a Maxwellian spectrum at five times the reference temperature and which peaks at the reference temperature. The group averages are determined by the scheme described below.

Recall that the Nordheim treatment is written to determine an average flux in a fuel lump that is part of a two-region system. The flux in the moderator is assumed to be asymptotic (viz., 1/E) which allows one to eliminate one of the two collision density equations.

In a high percentage of runs, cross sections are desired for use in a different geometry from that in which the Nordheim calculation is made, for example, as when a reactor pin is mocked and cross sections are wanted for a smeared representation of the lattice structure. This requires a "cell weighting" to be performed.

NITAWL-II accommodates "cell" and/or "zone" weighting in a very simple fashion.

Consider the defining equation for a cell-weighted cross section for a nuclide occurring in the fuel region:

$$\bar{N}\,\bar{\sigma}_g^{cell}\,\bar{\phi}_g^{cell}\,V_{cell} = \int_{Fuel} N(\bar{r})d\bar{r} \int_g dE\ \bar{\phi}^{Fuel}(E)\,\sigma(E)\ , \qquad \text{(F2.3.31)}$$

where

$N(\bar{r})$ is the number density in the fuel and is constant,

$\bar{\phi}^{Fuel}(E)$ is the flux-per-unit volume in the fuel as determined by the Nordheim treatment,

$\sigma(E)$ is the Doppler-broadened point cross section,

V_{cell} is the total volume of the cell,

$\bar{N}$ is the volume-averaged number density of the nuclide in the cell,

$\bar{\phi}_g^{cell}$ is the cell-averaged flux for group g,

$\bar{\sigma}_g^{cell}$ is the cross section required to preserve the reaction rate calculated on the right-hand side of the equation.

By definition,

$$\bar{N} = \frac{\int_{Fuel} N(\bar{r})d\bar{r} + \int_{Moderator} N(\bar{r})d\bar{r}}{\int_{cell} d\bar{r}} = V_F N_F / V_{cell}\ , \qquad \text{(F2.3.32)}$$

where V_F is the volume of the fuel region, and N_F is the atom density of the nuclide in the fuel region. (Note that it has been assumed that the nuclide for which a resonance calculation is being performed occurs only in the fuel region.) Likewise,

$$\bar{\phi}_g^{cell} = \frac{\int_g d\bar{E}\left[\int_{Fuel} dr\ \bar{\phi}^{Fuel}(E) + \int_{Mod} d\bar{r}\ \bar{\phi}^{Mod}(E)\right]}{V_{cell}}\ . \qquad \text{(F2.3.33)}$$

The assumption is then made that $\bar{\phi}^{Mod}$ 1/E consistent with the earlier assumption, such that

$$\bar{\phi}_g^{cell} = \int_g dE\ \bar{\phi}^{Fuel}(E)\,\frac{V_F}{V_{cell}} + \int_g \frac{dE}{E}\left(1 - \frac{V_F}{V_{cell}}\right)\ . \qquad \text{(F2.3.34)}$$

Substitution into Eq. (F2.3.31) ultimately yields

$$\bar{\sigma}_g^{cell} = \frac{\int_g dE\ \bar{\phi}^{Fuel}(E)\ \sigma(E)}{\bar{\phi}_g^{cell}}, \qquad \text{(F2.3.35)}$$

which is the expression calculated in NITAWL-II.

Note that if we define $G = \frac{V_F}{V_{cell}}$ in Eq. (F2.3.34), then

$$\bar{\phi}_g^{cell} = G \int_g dE\ \bar{\phi}^{Fuel}(E) + (1 - G)\,\Delta u_g, \qquad \text{(F2.3.36)}$$

where Δu_g is the lethargy width of group g. We can use the single parameter G—the volume fraction of the fuel lump in the cell—to determine either "cell-" or "zone-" weighted cross sections. (In the latter case, a value of G = 1.0 is used.) Note that this is the only use of this parameter in NITAWL-II.

In most cases, it is thought to be better to specify G = 1.0 and to perform an intermediate calculation (e.g., a simple 1-D S_n calculation) to perform "cell" weighting. The primary reasons are the following:

1. The Nordheim treatment only covers the resolved resonance region and, even here, only a part of the resonance range for a resonance.

2. Moderator nuclides also need a "cell" weighting, which will not be addressed by the Nordheim treatment.

Other approximations are needed when the break points for the Nordheim range fall within a group. In these cases, the flux in the fuel must be calculated over the entire energy group, when defining the denominator flux described by Eq. (F2.3.35). Here, the flux is assumed to be 1/E above 5 kT with a Maxwellian shape assumed below that point.

The integrations over $\bar{\phi}^{Fuel}(E)$ and $\bar{\phi}^{Fuel}\,\sigma(E)$ are performed analytically after assuming that both the flux and cross section are linear with lethargy. Since the Nordheim calculation is performed on a very fine equally spaced lethargy mesh, this integration scheme is very accurate and efficient.

The above discussion applies for the cross sections weighted over the spectrum determined for the problem. The cross sections at the reference temperature are weighted using exactly the same equations with the flux replaced by a 1/E flux tied to a Maxwellian spectrum. The output from the weighting calculation is the difference between the values weighted over the problem flux and the smooth flux.

F2.3.5.1 New Procedure for Referencing Shielded Cross-Section Values

In earlier versions of NITAWL, several special sets of cross sections were carried with resonance nuclides and were identified as follows:

MT	Value
1021	The 1/E averaged value of the n,γ cross sections over the energy regions for which the Nordheim calculation would be made.
1022	The 1/E averaged value of the n,f cross sections calculated as described above.
1023	The 1/E averaged value of the elastic scattering cross section over the full resonance range.

In this case, the "total values" in MT = 1, MT = 18, MT = 27, MT = 101, and MT = 102, corresponding to total, fission, absorption, capture, and n,γ, respectively, contained the weighted values for the cross sections for the energy range outside of the ranges over which the Nordheim calculation is made. The values for process identifiers (MT-numbers) correspond to those defined in ref. 11, in most cases.

This fit with a procedure which added the "shielded" value to the "total" values to define a final cross-section value. The special cross sections, MT = 1021 and MT = 1022, were only used when no resonance calculation was requested, thereby making a set of cross sections with infinite dilution values.

Elastic scattering was treated slightly differently in that MT = 1023 contained the total infinite dilution value, while MT = 2 data (elastic scattering) contained everything except the "bodies" of the resonances to be calculated by the Nordheim treatment.

The primary disadvantage of the treatment just described is that it requires the preprocessing code (in this case, XLACS) to understand enough about the Nordheim treatment to be able to know how to split the averages into the pieces described.

The present formulation of the Nordheim treatment references its shielded values to infinite dilution values, that is,

$$\sigma_{\text{final}} = \sigma_{\text{infinite dilution}} + \Delta\sigma \, .$$

The new procedure thereby relieves the basic processing code of having to know anything at all about the Nordheim treatment. It also means that one can introduce additional resonance data to the calculation, if it is necessary. An example of when this might be required is the case of including $\ell = 1$ resonance parameters in the Nordheim calculation, something not done previously with any SCALE libraries.

The new scheme does put an additional burden on the Nordheim treatment because it now must determine infinite-dilution averages. This process, however, is simple and straightforward as compared with that of determining self-shielded values.

In the new libraries, cross sections with MT numbers given by

$$3000 + \text{MT}$$

are used to store the reference infinite dilution values. For example, 3102 contains the infinite-dilution values for MT = 102. The values in MT = 102 are those determined by weighting the cross sections over the flux used in the basic processing of the data and will not be used unless the MT in the "3000" range is not present.

F2.3.6 UNRESOLVED RESONANCE CONTRIBUTIONS

NITAWL-II contains no provisions for performing an unresolved resonance calculation, as did its predecessors. In the SCALE system, this operation is typically performed by the BONAMI-S module.

F2.3.7 ESCAPE PROBABILITIES, POINT CROSS-SECTION FORMULATION, AND DOPPLER BROADENING

The first-flight escape probabilities appearing in Eq. (F2.2.1) and discussed in Sect. F2.2.2 are functions of geometry type and size as represented by a characteristic dimension, $\bar{a}$. Also, they are explicit functions of the mean-free path, λ, of the absorber material and implicit functions of energy through the inverse relationship between λ and $\Sigma_T(E)$. The analytic expressions developed by Case, deHoffman, and Placzek[7] for the escape probabilities for the slab, cylinder, and sphere are given by Eqs. (M7.A.18) through (M7.A.20) of Sect. M7.A.2 of the SCALE manual.

Earlier versions of NITAWL determined escape probabilities using algorithms programmed by Kuncir.[3] These allowed treating simple spheres, slabs, and cylinders. This version of NITAWL extends these capabilities by allowing one to treat annular systems.

As in most implementations, the escape probabilities are given as a function of $\bar{a}/\lambda$. For spheres, a function routine called P0SPH is called with two arguments, $\bar{a}/\lambda$ for the inner and outer radii of the shell, respectively. (Note that the inner radius is set to zero to treat a solid sphere.) The equations used in this case are those developed by Westfall[12] for use in the ROLAIDS module. For this, he defines the following terms:

P^+ = first-flight escape probability through the outer surface,

P^- = first-fight escape probability through the inner surface,

T^{OI} = first-flight transmission probability from the inner to the outer surface,

T^{IO} = first-flight transmission probability from the outer to the inner surface,

T^{OO} = first-flight transmission probability from the outer to the outer surface.

Define

$$R = \bar{a}/\lambda \ , \tag{F2.3.37}$$

and let R_1 be the value at the inner radius, while R_2 is the value for the outer radius.

It is shown that

$$P^+ = \frac{3R_2^2}{4(R_2^3 R_1^3)}\left[1 - T^{OO} - T^{IO}\right] , \tag{F2.3.38}$$

$$P^{-} = \frac{3R_1^2}{4(R_2^3 R_1^3)}[1 - T^{OI}] , \qquad \text{(F2.3.39)}$$

where

$$T^{OI} = \frac{1}{2R_1^2}\left\{(R_2 + R_1)^2 E_3(R_2 - R_1) - (R_2^2 - R_1^2) E_3\left(\sqrt{R_2^2 - R_1^2}\right)\right\}$$

$$+ \exp\left(-\sqrt{R_2^2 - R_1^2}\right)\left(\sqrt{R_2^2 - R_1^2} + 1\right) - \exp\left[-(R_2 - R_1)\right]$$

$$\left\{\sqrt{R^2 \times (R_2 - R_1 + 1)}\right\} , \qquad \text{(F2.3.40)}$$

$$T^{IO} = \left(\frac{R_1}{R_2}\right)^2 T^{OI} , \qquad \text{(F2.3.41)}$$

$$T^{\infty} = \frac{1}{2R_2^2}\left[1 - \exp\left(-2\sqrt{R_2^2 - R_1^2}\right)\left(1 + 2\sqrt{R_2^2 - R_1^2}\right)\right] . \qquad \text{(F2.3.42)}$$

E_3 is the third-order exponential integral function. For cylinders, the procedures developed by Kier and Robba[13] are used. These procedures have been programmed into function P0CYL, which has the same argument definitions as does P0SPH. This routine calls CYLPRB to pregenerate a table of escape probabilities. CYLPRB calls SHELC to generate transmission probabilities for cylindrical shells. The tabulations are used, except when $R_2 - R_1 > 8.0$, in which case an asymptotic expression is employed.

For slabs of thickness $\bar{a}$, the following expression is used:

$$P_0 = (1 - 2E_3(\bar{a}/\lambda))/(2\bar{a}/\lambda) . \qquad \text{(F2.3.43)}$$

The capture, fission, and scatter cross sections are calculated at each mesh energy, E, according to the single-level Breit-Wigner formulation as specified on pages D-1 through D-4 of the ENDF/B documentation.[11] The cross-section determination is done in subroutine RESOL with the Doppler shape functions $\psi(X_1,\xi)$ and $\chi(X_1,\xi)$ obtained with subroutine VOGAM as described below. The Doppler-broadened cross sections are given by the following formulas:

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

$$+ \frac{4\pi}{k^2} g \frac{\Gamma_n^\ell}{\Gamma}\frac{\sin 2\phi_\ell}{2}\chi(X_1,\xi) + \left(\frac{\Gamma_n^\ell}{\Gamma} - 2\sin^2\phi_\ell\right)\psi(X_1,\chi) , \qquad \text{(F2.3.44)}$$

$$\sigma_{n,\gamma}^{\ell}(E) = \frac{4\pi}{k^2} g \frac{\Gamma_n^{\ell}\Gamma_\gamma}{\Gamma^2} \psi(X_1,\xi) , \qquad \text{(F2.3.45)}$$

$$\sigma_{n,f}^{\ell}(E) = \frac{4\pi}{k^2} g \frac{\Gamma_n^{\ell}\Gamma_f}{\Gamma^2} \psi(X_1,\xi) , \qquad \text{(F2.3.46)}$$

where g is the statistical weight for the sequence of resonances. The RESOL algorithm treats up through $\ell = 4$ resonances. Spin-dependent quantities appearing in the equations are the neutron width, Γ_n^{ℓ}, and the phase shift ϕ_ℓ. These quantities are defined in terms of three basic parameters: the neutron wave number, k, given by

$$k = 2.196771 \times 10^{-3} * \sqrt{E} * (AWRI / (AWRI + 1.0)) , \qquad \text{(F2.3.47)}$$

where AWRI is the ratio of the mass of the isotope to that of a neutron; the effective scattering radius, â, as specified in the ENDF/B data; and the channel radius, a, given by

$$a = 0.123 * \sqrt[3]{AWRI} + 0.08 . \qquad \text{(F2.3.48)}$$

The phase shifts for the two spin states are determined as

$$\phi_0 = \hat{\rho} \qquad \text{(F2.3.49)}$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho} \qquad \text{(F2.3.50)}$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\left(\frac{3\hat{\rho}}{3 - \hat{\rho}^2}\right) \qquad \text{(F2.3.51)}$$

$$\phi_3 = \hat{\rho} - \tan^{-1}\left[\frac{\hat{\rho}(15 - \hat{\rho}^2)}{15 - 6\hat{\rho}^2}\right] \qquad \text{(F2.3.52)}$$

$$\phi_4 = \hat{\rho} - \tan^{-1}\left[\frac{\hat{\rho}(105 - 10\hat{\rho}^2)}{105 - 45\hat{\rho}^2 + \hat{\rho}^3}\right], \qquad \text{(F2.3.53)}$$

where

$$\hat{\rho} = k\hat{a} .$$

Additional quantities used in determining the spin-dependent neutron widths are the penetration factors, P_ℓ, given by

$$P_0 = \rho \tag{F2.3.54}$$

$$P_1 = \rho^3/(1 + \rho^2) \tag{F2.3.55}$$

$$P_2 = \rho^5/(9 + 3\rho^2 + \rho^4) \tag{F2.3.56}$$

$$P_3 = \rho^7/(225 + 45\rho^2 + 6\rho^4 + \rho^6) \tag{F2.3.57}$$

$$P_4 = \rho^9/(11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8) , \tag{F2.3.58}$$

where

$$\rho = ka .$$

The spin-dependent neutron width is then obtained from the ENDF/B specified neutron width, Γ_n, by the ratio

$$\Gamma_n^\ell = P_\ell(E)\,\Gamma_n/P_\ell(E_0) , \tag{F2.3.59}$$

where the penetration factors are evaluated at the neutron energy, E, and the specified resonance base energy, E_0. Note that the dependence of the penetration factors on energy arises through the definitions of ρ and k.

Before proceeding with the discussion of Doppler broadening, it is appropriate to introduce one additional spin-dependent quantity, the resonance energy shift factor, S_ℓ. The effective resonance energy, E'_r, is related to the specified resonance base energy, E_0, by

$$E'_r = E_0 + [S_\ell(E_0) - S_\ell(E)]\Gamma_n/[2P_\ell(E_0)] . \tag{F2.3.60}$$

The shift factors appearing in Eq. (F2.3.88) are given by

$$S_0 = 0 \tag{F2.3.61}$$

$$S_1 = \frac{-1}{(1 + \rho^2)} \tag{F2.3.62}$$

$$S_2 = -\frac{(18 + 3\rho^2)}{(9 + 3\rho^2 + \rho^4)} \tag{F2.3.63}$$

$$S_3 = -\frac{(675 + 90\rho^2 + 6\rho^4)}{(225 + 45\rho^2 + 6\rho^4 + \rho^6)} \qquad \text{(F2.3.64)}$$

$$S_4 = -\frac{(44100 + 4725\,\rho^2 + 270\,\rho^4 + 10\,\rho^6)}{(11025 + 1575\,\rho^2 + 135\,\rho^4 + 10\,\rho^6 + \rho^8)} . \qquad \text{(F2.3.65)}$$

Thus, for $\ell = 0$, E'_r corresponds simply to E_o.

With the assumption of a Maxwellian distribution of target nuclei velocities, the Doppler shape functions are defined as

$$\psi(X_1,\xi) = \xi/(2\sqrt{\pi})\int_{-\infty}^{\infty}\exp\left[-(\xi/2)^2(X_1 - Y_1)^2\right](1 + Y_1^2)^{-1}dY_1 , \qquad \text{(F2.3.66)}$$

and

$$\chi(X_1,\xi) = \xi/\sqrt{\pi}\int_{-\infty}^{\infty}\exp\left[-(\xi/2)^2(X_1 - Y_1)^2\right]Y_1(1 + Y_1^2)^{-1}dY_1 , \qquad \text{(F2.3.67)}$$

where

$$X_1 = 2(E - E'_r)/\Gamma ,$$

and

$$\xi = \Gamma/\Gamma_0 = \Gamma\sqrt{AWRI\,/(4E'_r kT)} .$$

The integration over Y_1 accounts for the variation in target nuclei velocities.

The algorithm contained in VOGAM for calculating $\psi(X_1,\xi)$ and $\chi(X_1,\xi)$ was developed by J. H. Marable of Oak Ridge National Laboratory in the late 1960s. The algorithm contains three alternative procedures:

1. Asymptotic Series Expansion,
2. Taylor Series Expansion, and
3. Rational Approximation.

The numerical analysis associated with the Asymptotic and Taylor Series Expansions can be found in Abramowitz and Stegun.[14] The Rational Approximation is due to Adler and Naliboff.[15] For any particular set of input variables (X_1,ξ), the choice of which procedure is applied depends upon the value of a test parameter, T, defined as

$$T = \frac{\xi^2}{4}(X_1^2 + 1) . \qquad \text{(F2.3.68)}$$

For $T \leq 0.3469175$

The Taylor Series Expansion is applied.

For $0.3469175 < T < 78.50045$

The Rational Approximation is applied.

For $78.50045 \leq T < 1.342177 \times 10^8$

The Asymptotic Series Expansion is applied.

For $T \geq 1.342177 \times 10^8$

$$\psi(X_1, \xi) = \frac{1}{(1 + X_1^2)}$$

$$\chi(X_1, \xi) = \frac{2X_1}{(1 + X_1^2)} .$$

Also, depending upon where the value of T falls within the ranges defined above, the Asymptotic and Taylor Series solutions may include terms up to the fifth order in the independent variables x and y. These terms are summed as

$$T_1 = \frac{\xi}{2}[a_1 + a_2x + a_3r + a_4(r - 2y^2)x + a_5(2xy + r)(r - 2xy) + a_6((2xy + r)(r - 2xy) - 4ry^2)x] , \quad \text{(F2.3.69)}$$

and

$$T_2 = y\frac{\xi}{2}[a_2 + b_3x + a_4(r + 2x^2) + b_5r + a_6(4rx^2 + (2xy + r)(r - 2xy))] , \quad \text{(F2.3.70)}$$

where $r = x^2 + y^2$, the constant coefficients are given in Table F2.2.4, and x and y are defined below for each solution.

Table F2.2.4 Coefficients for the Asymptotic and Taylor Series Solutions

Coefficient	Asymptotic series	Taylor series
a_1	1.0	2.0
a_2	0.5	0.6666667
a_3	0.75	0.2
a_4	1.875	0.04761705
a_5	6.5625	0.00925926
a_6	29.53125	0.00151515
b_3	1.5	0.4
b_5	26.25	0.03703704

The Taylor Series solution is given by

$$\psi(X_1,\xi) = \frac{\xi}{2} e^{-x}[(T_1X_1 - T_2)\sin(y) - (T_2X_1 + T_1 - \sqrt{\pi})\cos(y)] , \qquad \text{(F2.3.71)}$$

and

$$\chi(X_1,\xi) = \xi e^{-x}[(T_1X_1 - T_2)\cos(y) + (T_2X_1 + T_1 - \sqrt{\pi})\sin(y)] , \qquad \text{(F2.3.72)}$$

where

$$x = \frac{\xi^2}{4}(X_1^2 - 1)$$

and

$$y = \frac{X_1\xi^2}{2} .$$

The Asymptotic Series solution is given by

$$\psi(X_1,\xi) = \frac{\xi}{2T}[T_1 - T_2X_1] , \qquad \text{(F2.3.73)}$$

and

$$\chi(X_1,\xi) = \frac{\xi}{T}[T_2 - T_1X_1] , \qquad \text{(F2.3.74)}$$

where

$$x = \frac{4}{\xi^2}\frac{(X_1^2 - 1)}{(X_1^2 + 1)^2}$$

and

$$y = \frac{-8}{\xi^2}\frac{X_1}{(X_1^2 + 1)^2} .$$

The rational approximation solution is given by

$$\psi(X_1,\xi) = (\xi/2)\, C_1C_2/(C_1^2 + X_1^2)$$
$$- [2(C_6 + C_5(C_3 + \xi/2))((C_3 + \xi/2)^2 + C_4 - (X_1\xi/2)^2) + C_5(C_3 + \xi/2)(X_1\xi)^2]/$$
$$[((C_3 + \xi/2)^2 + C_4 - (X_1\xi/2)^2)^2 + (C_3 + \xi/2)^2(X_1\xi)^2]$$
$$- [2(C_{10} + C_9(C_7 + \xi/2))((C_7 + \xi/2)^2 + C_8 - (X_1\xi/2)^2) + C_9(C_7 + \xi/2)(X_1\xi)^2]/$$
$$[((C_7 + \xi/2)^2 + C_8 - (X_1\xi/2)^2)^2 + (C_7 + \xi/2)^2(X_1\xi)^2] , \qquad \text{(F2.3.75)}$$

and

$$\chi(X_1,\xi) = X_1\, 2C_2/(C_1^2 + X_1^2)$$
$$- \xi^2[2(C_6 + C_5(C_3 + \xi/2))(C_3 + \xi/2) - C_5(C_3 + \xi/2)^2 + C_4 - (X_1\xi/2)^2]/$$
$$[((C_3 + \xi/2)^2 + C_4 - (X_1\xi/2)^2)^2 + (C_3 + \xi/2)^2(X_1\xi)^2]$$
$$- \xi^2[2(C_{10} + C_9(C_7 + \xi/2))(C_7 + \xi/2) - C_9((C_7 + \xi/2)^2 + C_8 - (X_1\xi/2)^2)]/$$
$$[((C_7 + \xi/2)^2 + C_8 - (X_1\xi/2)^2)^2 + (C_7 + \xi/2)^2(X_1\xi)^2] \qquad \text{(F2.3.76)}$$

where the constants C_1, C_2, ... C_{10} are given in Table F2.2.5.

Table F2.2.5 Constants for the Rational Approximation Solution

C_1	0.93530073218	C_6	-0.4375413094
C_2	1.0293006226	C_7	0.83026130674
C_3	0.91274177018	C_8	2.6577963326
C_4	0.5966313823	C_9	0.07294699933
C_5	-0.05850576307	C_{10}	-0.03664708606

Comparisons of VOGAM values for $\psi(X_1,\xi)$ and $\chi(X_1,\xi)$ with values obtained by integrating Eqs. (F2.3.66) and (F2.3.67) over numerical quadrature have demonstrated maximum deviations of a few tenths of 1%. Thus, the VOGAM algorithm is an accurate and efficient means of obtaining the Doppler-shape functions.

F2.4 AMPX LIBRARY FORMAT CONVERSION

One major function of NITAWL-II is to convert data from an AMPX master library into the AMPX working library format.

An AMPX master library is not structured for direct use in a multigroup particle transport calculation. The intent is to provide a means to present a library that has the potential of being truly problem-independent which can be tailored at run-time for a particular problem. The library also carries data at a sufficient level of detail to allow satisfying many of the less-common, but very powerful, analyses such as cross-section sensitivity studies and coupled neutron-gamma transport calculations. The libraries can, in some cases, allow resonance self-shielding to be performed using the Nordheim method, the Bondarenko method, or an integral transport calculation with many spatial zones. Temperature dependence of data is allowed. Any number of scattering processes can be included to any degree of anisotropic representation. In short, there is far too much detail to require transport codes to process this library.

NITAWL-II serves to process and combine the data mentioned above into a form ready for use by most particle transport programs. Provisions are included to allow performing a Nordheim integral treatment resonance self-shielding calculation for those nuclides with resonance parameters supplied as part of the data. The final output is an AMPX working library.

The AMPX working library contains two types of data: first, group-averaged cross sections for an arbitrary number of processes for neutrons and/or gamma rays and, second, total transfer matrices for neutrons and/or gamma rays.

Many operations may be required in order to produce the working library, as will be evidenced when the library formats are described later in this section.

In the case of Bondarenko data, NITAWL-II simply skips it. Processing of these data is provided in BONAMI-S, discussed in Sect. F1 of the SCALE manual.

The master library can contain resonance parameter data. Processing these data has been described at length in Sect. F2.3. The output is a set of group-averaged values for (n, γ) capture, fission, and elastic scattering. These values are passed for substitution into appropriate positions later in the processing. This requires the adjustment of many "total" values, such as absorption, capture, etc., to ensure consistency.

The final operation is to add together all the transfer matrices in order to form a total transfer matrix. This requires several special operations. In many cases, the transfer matrices are temperature-dependent. NITAWL-II picks the matrix whose temperature is closest to that specified for the nuclide (i.e., no interpolation is performed at present). For resonance nuclides, the elastic scattering matrix is scaled uniformly to make the matrix consistent with the self-shielded values. The $P_\ell(\ell > 0)$ matrices are scaled by the amount required for the P_0 matrix. For processes involving multiple-exit neutrons [e.g., (n,2n), (n,3n), etc.] NITAWL-II multiplies by the appropriate multiplicity before adding to the total transfer matrix. In the case of coupled neutron-gamma libraries, gamma yields are sometimes expressed in "yield" units, thereby requiring a multiplication by a cross section before their introduction into the total transfer matrix. (This scheme allows one to produce self-shielded gamma production cross sections.) After everything is added together, provisions are included to compress out most zero and/or nonexistent elements in the transfer arrays prior to placing them on the working library.

Descriptions of the AMPX master and working library formats are given on the following pages.

The AMPX multigroup formats have been designed to allow a generality paralleling that of the ENDF/B point libraries. For example:

1. The formats can accommodate neutron libraries, gamma libraries, or coupled neutron-gamma libraries.

2. An arbitrary number of reaction cross sections can be included with ENDF/B identifiers used for processes, where possible.

3. An arbitrary order of anisotropy can be presented which can vary from nuclide to nuclide or even from process to process, in the case of the master library.

4. Temperature dependence is allowed on the master library.

5. Resonance parameters may be included on the master library for use in Nordheim resolved resonance calculations and/or in an unresolved resonance calculation.

6. The master library can contain Bondarenko data for resonance self-shielding by BONAMI-S (cf., Sect. F1).

7. The master library can include scattering matrix data for an arbitrary number of processes.

In the case of the resonance data, partial energy range data can be specified. For example, on some of the SCALE libraries, the Bondarenko data are only for the unresolved region, which will vary from nuclide to nuclide.

Potentially, the most space-consuming data on a cross-section library are the transfer matrix data. AMPX uses so-called "magic-word" arrays for these data which help to eliminate zero and/or impossible data elements. This procedure is especially important for the master library, where the library may contain data for ~50 separate processes represented to an arbitrary level of anisotropy.

The two formats are written using a combination of seven kinds of information, each of which has one or more record types associated with it:

1. Header information—written on the front of the library to specify the number of neutron and/or gamma groups, the number of nuclides, etc., contained in the library. (Record Type 1)

2. Energy structure information—contains the group boundaries. (Record Type 2)

3. Nuclide directory information—50 words that give a title for the nuclide, along with other parameters that specify the kinds of information included for the nuclide, such as number of records in the library for the nuclide and how much neutron and gamma data are given. (Record Type 3)

4. Resonance parameter data—provisions for resolved resonance parameters in the single-level Breit-Wigner or multilevel Breit-Wigner (SLBW or MLBW) formats. (Record Type 4)

5. Bondarenko data—four record types are used for this information:

    a. A record that gives the values of σ_0 and T at which the factors are tabulated, along with cutoff energies for the Bondarenko calculation. The parameter σ_0 is the cross-section value for all nuclides mixed with the nuclide being calculated, and T is the temperature value. (Record Type 5)

    b. A directory record containing information about the specific processes for which the Bondarenko factor data apply, such as the process, the energy groups for which data are given, etc. (Record Type 6)

    c. A record containing infinite dilution values for a process. (Record Type 7)

d. A record containing the Bondarenko factors for a process. (Record Type 8)

6. A record containing average cross sections by process. (Record Type 9)

7. Three record types are used to present transfer matrices:

   a. A directory record that specifies the processes, orders of anisotropy, lengths, units, etc. (Record Type 10)

   b. A record to specify temperatures when the matrices are temperature dependent. (Record Type 11)

   c. A "magic-word" record to store a transfer matrix. (Record Type 12)

   A discussion of the structure of each of the various record types follows.

Record Type 1 (Header Record)

The header record is the first record on a master and a working library and always contains 110 words:

1. IDTAPE - An identification number for the library.

2. NNUC - The number of sets of data on the library.

3. IGM - The number of neutron energy groups on the library.

4. IFTG - The first thermal neutron group on the library (i.e., the first group that receives an upscatter source).

5. MSN - Zero.

6. IPM - The number of gamma-ray energy groups on the library.

7. I1 - Zero.

8. I2 - (0/1 = no/yes) A trigger that specifies that this library was produced by weighting a working library in the XSDRNPM module.

9. I3 - Zero.

10. I4 - Zero.

11-110. (TITLE(I), I=1,100) - 100 words of text describing the cross-section library.

Record Type 2 (Energy Boundaries)

This record is on both a master and a working library and specifies the energy boundaries in eV of the neutron groups and/or gamma groups, followed by the corresponding lethargy boundaries. The energy boundaries are arranged in descending order, followed by the lethargy boundaries in ascending order. The "lethargy zero" is taken at 10 MeV. The structure is

$$(EB(I),I=1,IGP), (UB(I),I=1,IGP),$$

where IGP is the number of groups plus 1.

Record Type 3 (Cross-Section Set Directory Record)

Each set of data on a master or working library has a 50-word directory record that specifies certain parameters needed to determine dimensions required to process the data and to describe the make-up of the set of data. The table on the following page describes these data.

Note that the 50-word records are made up of integer, character, and floating-point words. Words 1 to 18 and 49 are character data. Words 29, 30, 34, 35, and 43 are floating point. All other words are integers. For both types of libraries, many parameters may have no meaningful interpretation for a particular set of data. This situation is especially true of the working library; for example, words 20, 21, 22, 25, and 26 only have meaning if the working library has been produced by weighting a previous working library. Zero values will be used when a parameter is not applicable.

Record Type 4 (Resonance Parameters)

This record is present only when either the number of six-word resonance sets, NRES, or the number of unresolved energy points, NUNR, is nonzero. Its length is

$$9 + 6*NRES + NUNR.$$

All values are in floating point.

The first nine words contain parameters used in both the resolved and unresolved resonance calculations

1. A, the mass ratio for the isotope or mixture of isotopes;

2. σ_P, the potential scattering cross section;

3. g, the average statistical factor in the unresolved region;

4. NRES, the number of six-parameter resonance sets;

5. s, a factor used in the Nordheim calculation to determine the range over which the calculation will be made (cf., Sect. F2.3.3);

6. <D>, the average level energy spacing for the $\ell = 0$ unresolved sequence which will be calculated;

7. $\langle\Gamma_n^0\rangle$, the average unresolved neutron width;

8. $\langle\Gamma_\gamma\rangle$, the average unresolved gamma width;

9. $\langle\Gamma_f\rangle$, the average unresolved fission width.

The next 6*NRES words consist of six-word sets of data used in the Nordheim calculation.

1. Zero;

2. NBLK, the number of blocks of resolved data;

3. Zero;

4. Zero;

5. TREF, the reference temperature at which the infinite dilution arrays on this library were calculated;

6. Zero

Following these six words are NBLK six-word groups that are used to specify information concerning blocks of resonance data that apply to, for example, different isotopes, different energy regions, different kinds of data (s-wave or p-wave resonances), etc. These groups are stacked as follows:

1. AWRI, the mass ratio associated with the block of data;

2. ABUN, the abundance for the block of data;

3. NRE, the number of resonances in the block;

4. ℓ, the value of spin for the resonances in the block;

5. EL, the low-energy cut-off for resonances in the block;

6. EH, the upper energy cut-off for resonances in the block;

.
.
.

Word(s)	Master Library	Working Library
1-18	18 words of text describing the set	18 words of text describing the set
19	Identifier of the set	Identifier of the set
20	Number of 6-parameter sets of resolved resonance data	Identifier of the set from which this set derived
21	Number of energies at which to evaluate unresolved values	Zone number in which the nuclide occurred
22	Number of neutron processes for which group-averaged values are given (temperature independent)	Number of zones in problem which produced this set
23	Number of neutron processes with scattering arrays	Length of P_0 total scattering matrix
24	Zero	Order of expansion of total scattering matrix
25	Number of gamma processes for which group-averaged values are given	Sequence of this set in all zone-weighted sets
26	Number of gamma processes with scattering arrays	Number of zone-weighted sets for this nuclide
27	Number of neutron-to-gamma processes	Maximum length of any scattering array in with scattering arrays
28	(Maximum order of scattering)*32768 + (total number of separate scattering arrays for this set)	Number of neutron processes which have group-averaged values
29	A - neutron equivalent mass number	A - neutron equivalent mass number
30	ZA - 1000*Z + A	ZA - 1000*Z + A
31	Zero	Zero
32	Zero	Zero
33	Zero	Zero
34	Power per fission in w-s/fission	Power per fission in watt-sec/fission
35	Energy release per capture in w-s/capture	Energy release per capture in w-s/capture
36	Maximum length of any scattering array in the set	Zero
37	Number of sets of Bondarenko data	Zero
38	Number of σ_0's in Bondarenko data	Zero
39	Number of T's in Bondarenko data	Zero
40	Maximum number of groups in Bondarenko data	Zero
41	Zero	Number of gamma processes that have group-averaged values
42	Zero	Zero
43	σ_p - potential scattering cross section	Zero
44	Zero	Zero
45	ENDF MAT for fast neutron data	ENDF MAT for fast neutron data
46	ENDF MAT for thermal neutron data	ENDF MAT for thermal neutron data
47	ENDF MAT for gamma data	ENDF MAT for gamma data
48	ENDF MAT for gamma production data	ENDF MAT for gamma production data
49	Nuclide symbol (Text)	Nuclide symbol (Text)
50	Number of records in this set	Number of records in this set

After these NBLK groups of six words comes the six-word sets of resonance parameters arranged as follows:

1. E_0, the resonance energy,
2. Γ_n, the neutron width of the resonance,
3. Γ_γ, the gamma width of the resonance,
4. Γ_f, the fission width of the resonance,
5. r, a factor used in the Nordheim treatment for determining the range of calculation,
6. g, the statistical factor for the resonance.

The following chart illustrates the structure just described schematically:

	1	2	3	4	5	6
	0	NBLK	0	0	T_{ref}	0
	$AWRI_1$	$ABUN_1$	NRE_1	ℓ_1	EL_1	EH_1
	$AWRI_2$	$ABUN_2$	NRE_2	ℓ_2	EL_2	EH_2
	.					
	.					
	.					
	$AWRI_{NBLK}$	$ABUN_{NBLK}$	NRE_{NBLK}	ℓ_{NBLK}	EL_{NBLK}	EH_{NBLK}
	E_0	Γ_n	Γ_γ	Γ_f	r	g
	.	.	.	.	.	.
first	.	.	.	.	.	.
block	.	.	.	.	.	.

After the resolved resonance parameters, the points at which the unresolved cross section should be evaluated are specified. There are NUNR of these points arranged low-to-high in energy:

(EUNR(I), I=1, NUNR)

Record Type 5 (First Record of Bondarenko Block)

This record is used to specify the σ_0 and temperature values at which all Bondarenko factors for the nuclide will be presented. It also specifies the upper and lower energies for which factors can apply in the case

where they do not span all energy groups. The number of σ_0 values, NSIG0, is specified in the 38th word in the set directory, and the 39th word specifies the number of temperatures, NT. The record structure is

$$(\sigma_0(I), I=1, NSIG0), (T(I), I=1, NT), ELO, EHI .$$

The σ_0 values can either ascend or descend; the temperatures are expressed in Kelvin in ascending order. The parameter σ_0 is the cross-section value for the other nuclides mixed with a nuclide in a particular situation.

Record Type 6 (Directory for Bondarenko Data)

This record type is used to specify the processes that have Bondarenko data in the set. Its length is six times NBOND, the number of Bondarenko processes, specified in the 37th word in the set directory. The structure is the following:

(MT(I), I=1, NBOND);
(NF(I), I=1, NBOND);
(NL(I), I=1, NBOND);
(ORDER(I), I=1, NBOND);
(IOFF(I), I=1, NBOND);
(NZ(I), I=1, NBOND).

The parameters have the following interpretation: MT is the identifier of the process (e.g., MT = 2 is for elastic scattering as in ENDF/B). NF is the number of the first energy group for which parameters are given. NL is the last group for which parameters are given. ORDER is used to specify the order of the scattering matrix in the event it is to be self-shielded. IOFF is the offset from the "magic-word" in the transfer matrices; for example, for elastic scattering, the first word after the magic-word is generally the within-group term such that IOFF=1 would specify the shielding for the within-group terms. (This parameter will be clearer when the transfer matrix description—record type 12—is read.) NZ is presently unused and has a zero value.

Record Type 7 (Infinite Dilution Values for Bondarenko Data)

Each process that has Bondarenko data has one of these records which contains the infinite-dilution values for the process. Its structure is

$$(\sigma^{\infty}(I), I=NF, NL) ,$$

where NF and NL are the first and last groups with data for the process.

Record Type 8 (Bondarenko Factors)

This record is a three-dimensional (3-D) array and contains the Bondarenko factors for a process. Its structure is

$$(((BF(I,J,K), I=1, NSIGO), J=1, NT), K=NF, NL) .$$

Record Type 9 (Temperature-Independent Average Cross Sections)

This record type is used to present average cross sections (sometimes called 1-D cross sections) on the library.

Its structure is

MT_1, (σ_1(I), I=1, IGM)
MT_2, (σ_2(I), I=1, IGM)
.
.
.
MT_{LAST}, (σ_{LAST}(I), I=1, IGM) ,

where the MTs are the process identifiers, and the cross sections, σ, are given for all groups. (Note that the MTs are given as floating-point numbers.)

Record Type 10 (Scattering Matrix Directory)

An AMPX master library always provides a directory that identifies the scattering matrices which are given for a nuclide. The structure is

(MT(I), I=1, N2D),
(L(I), I=1, N2D),
(NL(I), I=1, N2D),
(NT(I), I=1, N2D),

where N2D is the number of scattering (2-D) processes, MT is the process identifier, L is the maximum length of any of the scattering matrices for the process, NL is the order of Legendre fit to the scattering matrix, and NT is a parameter whose definition depends on the type of data (whether neutron, gamma production, or gamma) given as follows:

1. For neutron-neutron data, NT is the number of temperatures at which scattering matrices are given.

2. For gamma production data, NT is zero if the data are in yield units and is unity if they are in cross-section units.

3. For gamma-gamma data, NT is zero.

Record Type 11 (Scattering Matrix Temperatures)

This record type is only used on a master library and specifies the temperatures (in eV) of the scattering matrices. It is only used for neutron-neutron data and is given when NT > 0 (see Record Type 10). The temperatures are in ascending order as follows:

(T(I), I=1, NT)

Record Type 12 (Scattering Matrix)

This record type is used to store scattering-matrix data (sometimes called 2-D data). As will be illustrated, it has provisions for truncating zero and/or impossible elements from the array. It exists in two forms: (1) a self-defining form used for gamma production data on a master library and for all scattering matrices on a working library, and (2) a form that is not self-defining. The only difference is that the self-defining form specifies the length as the first word, while the other does not; that is,

$$L, (X(I), I=1, L)$$

or

$$(X(I), I=1, L) .$$

The structure of the X-array is as follows:

Magic word for a group,
Terms for scattering to the group,
Magic word for the next group,
Terms for scattering to this group,
Etc., etc.

In some cases, a negative or zero magic-word is used to specify the end of data in the record.

A "magic-word" is used to define:

1. the sink group number, III,
2. the first group number, JJJ, which scatters to this group,
3. the last group number, KKK, which scatters to this group.

The magic-word is then defined as

$$MW = 1000000*JJJ + 1000*KKK + III ,$$

such that it is composed of three 3-digit integers:

$$MW : JJJKKKIII .$$

The scattering terms below a "magic-word" are in reverse ordering (following typical practice for transport theory programs); that is, the scattering term for scattering from the last group is first, etc.:

MW for group III
σ(KKK→III)
σ(KKK-1→III)
.
.

σ(JJJ→III)

The scattering matrix record will contain one P_ℓ matrix for a process.

Consider an elastic scattering matrix for hydrogen which will be a full triangular matrix and assume three energy groups. The scattering matrix will look as follows:

1001001
σ(1→1)
1002002
σ(2→2)
σ(1→2)
1003003
σ(3→3)
σ(2→3)
σ(1→3)

Note that the record is a mixture of integer and floating-point terms.

AMPX Master Library Format

The overall structure of an AMPX master library is given as follows:

	Record type
Header record	1
Nuclide directory (one record per nuclide)	3
Neutron energy boundaries	2
Gamma energy boundaries	2
Records for nuclide 1	
Records for nuclide 2	
Etc.	

The structure of the records of a nuclide is:

	Record type
Nuclide directory record	3
Bondarenko data (one record per nuclide)	5,6,7,8
Resonance parameter data	4
Temperature-independent, group-averaged neutron cross sections	9
Scattering matrix data for neutrons	10,11,12
Group-averaged gamma cross sections	9
Scattering matrix data for gammas	10,12

The internal structure for Bondarenko data is:

	Record type
$(\sigma_0(I),I=1,NSIGO),(T(J),J=1,NT),EL,EH$	5
Bondarenko data directory (MT(I),I=1,NBOND), (NF(I),I=1,NBOND), (NL(I),I=1,NBOND), (ORDER(I),I=1,NBOND), (IOFF(I),I=1,NBOND), (NZ(I),I=1,NBOND)	6
The following records are given in pairs for all NBOND Bondarenko processes.	
Infinite dilution values $(\sigma^{\infty}(i),I=NF,NL)$	7
Bondarenko factors (((BF(I,J,K),I=1,,NSIGO),J=1,NT),K=NF,NL)	8

The internal structure of the scattering matrix data for neutrons is:

	Record type
Scattering matrix directory (MT(I),I=1,N2D), (L(I),I=1,N2D), (NL(II),I=1,N2D), (NT(I),I-1,N2D)	10
The following structure is repeated N2D times.	
Temperature values (NT>0) (T(I),I=1,NT)	11
The following record is repeated MAX(1,NT)*(NL+1) times.	
Scattering matrix (X(I),I=1,L)	12

The internal structure for gamma production scattering is:

Scattering matrix directory (MT(I),I=1,N2D), (L(I),I=1,N2D), (NL(I),I=1,N2D)	10
For each process, I=1, N2D, the following record type is given NL+1 times corresponding to the P_0, P, ..., P_{NL} matrices.	
Self-defining scattering matrix length LENGTH,(X(I),I=1,LENGTH)	12

The internal structure for gamma-gamma scattering is:

Scattering matrix directory (MT(I),I=1,N2D), (L(I),I=1,N2D), (NL(I),I=1,N2D), (NT(I),I=1,N2D)	10
For each process, I=1, N2D, the following record type is given NL+1 times corresponding to the P_0, P_1, ..., P_{NL} matrices.	
Scattering matrix (X(I),I=1,L)	12

AMPX Working-Library Format

The overall structure of a working library is given below:

	Record type
Header records	1
Neutron energy boundaries	2
Gamma energy boundaries	2
Nuclide directory (one record per nuclide)	3
Records for nuclide 1	
Records for nuclide 2	
Etc.	

The structure of the records for a nuclide is:

	Record type
Nuclide directory record	3
Group-averaged neutron cross sections	9
Group-averaged gamma cross sections	9
The P_0, P_1, ..., P_{NL} total scattering matrices are presented in self-defining records.	
L,(X(I),I=1,L)	12

F2.4.1 DIFFERENCES BETWEEN THE AMPX MASTER LIBRARIES USED BY NITAWL-II AND PREVIOUS VERSIONS

The format of the master library used in NITAWL-II is identical to that used by previous versions of the code. However, there are several differences, as discussed in Sect. F2.3.5, which redefine some of the parameters within the library.

One obvious difference is that the new libraries will contain no unresolved resonance data, since there is no unresolved calculation in NITAWL-II.

In the group-averaged parameters, the values are now expected to be infinite dilution values and not background values as in earlier versions.

For those who wish to make use of an earlier AMPX master library in NITAWL-II, a simple conversion program called CORECTOL has been developed (see Sect. M15.6).

F2.5 SUMMARY OF FUNCTIONS BY SUBPROGRAM

On the following pages are descriptions of all subprograms written specifically for NITAWL-II. All are written in FORTRAN. Descriptions of library subprograms shared by more than one SCALE module are given in Sect. M2 of this document. These routines are identified by an asterisk.

F2.5.1 CRRCT

CALLING SEQUENCE:

CALL CRRCT (CX, RSA, RSN, RSS, IGP, N1D, IFTG, NRES, SS)

FUNCTION:

CRRCT is used to correct the initial infinite dilution values with self-shielded values generated by the Nordheim resonance treatment and the unresolved treatment. It also must make changes to ensure consistency of all "total" values such as the total values, capture values, absorption values, etc. In the case of resonance nuclides that bypass the resonance calculation, this routine must perform some summing operations in order to obtain complete infinite dilution values.

ARGUMENTS:

CX is the original unshielded cross-section array. It is dimensioned by (IGP, N1D).

RSA contains the difference between the resonance self-shielded values of the absorption cross section and the infinite dilution average of the absorption cross section.

RSN contains the difference between the resonance self-shielded values of the fission cross section and the infinite dilution average of the fission cross section.

RSS contains the difference between the resonance self-shielded values of the elastic scattering cross section, excluding the potential value and the infinite dilution average.

IGP is the number of energy groups plus 1.

N1D is the number of separate processes included in the CX array.

IFTG is the first thermal group.

NRES is a trigger on whether or not a resonance calculation is performed. It is unity if so, and zero otherwise.

SS is an array that returns the final self-shielded elastic scattering values for other uses in NITAWL-II.

F2.5.2 CXRT

CALLING SEQUENCE:

CALL CXRT (CX, N1D, XE, IFTG, IGP, IGM, RSS)

FUNCTION:

CXRT is used to correct the neutron elastic scattering and total cross sections to ensure consistency with the thermal matrix, which may vary as a function of temperature.

ARGUMENTS:

CX	is the 1-D cross-section array and is dimensioned (IGP, N1D).
N1D	is the number of processes included in the CX array.
XE	is the sum of the elastic (MT=2) and the thermal (MT=1007 and 1008) average cross sections by group.
IFTG	is the first thermal energy group.
IGP	is the number of neutron energy groups plus 1.
IGM	is the number of neutron energy groups.
RSS	is an array of self-shielded elastic cross sections from the Nordheim treatment.

F2.5.3 CYLPRB

CALLING SEQUENCE:

CALL CYLPRB (RO, RI)

FUNCTION:

CYLPRB is used to generate tables of transmission probabilities that are subsequently used to generate escape probabilities for cylindrical shells. SHELC is called to generate transmission probabilities.

ARGUMENTS:

RO is the value of $\bar{a}/\lambda$ for the outer radius.

RI is the value of $\bar{a}/\lambda$ for the inner radius.

F2.5.4 FOLD

CALLING SEQUENCE:

CALL FOLD (CX, L, X, IGM)

FUNCTION:

FOLD is provided for the case in which gamma production matrices are expressed in yield units, thereby requiring a multiplication by an average cross section to obtain "cross section" units:

$$\sigma(\text{neutron to gamma}) = \sigma(\text{neutron}) \text{ yield (neutron to gamma)}.$$

ARGUMENTS:

CX	is the transfer matrix array (see Sect. F2.4).
L	is the length of the transfer matrix.
X	is an array of the averaged cross sections.
IGM	is the number of neutron energy groups.

SUBROUTINES CALLED:

MGCWRD*

F2.5.5 GRID

CALLING SEQUENCE:

CALL GRID (EZERO, GAMN, GMGM, GFG, R, GAMMA, EONE, EPSIL, SIGOH, XI, MESH, AID, SPIN, JPRINT)

FUNCTION:

GRID performs several operations to determine constants used in the Nordheim calculation:

1. It determines $\Gamma_t = \Gamma_n + \Gamma_\gamma + \Gamma_f$.

2. It determines $\Gamma_a = \Gamma_\gamma + \Gamma_f$.

3. It replaces Γ_f with $\Gamma_f = \Gamma_f/\Gamma_a$.

4. It calculated σ_0 for each resonance.

5. It determines the mesh spacing, ϵ, the number of points in the mesh, and the upper energy of the Nordheim calculation for each resolved resonance.

5. It determines ξ for each resonance.

ARGUMENTS:

EZERO is an array of resonance energies.

GAMN is an array of neutron widths for each resonance.

GMGM is an array of gamma widths for each resonance.

GFG is an array of fission widths for each resonance.

R is an array for the r-factors (see Sect. F2.3.3) for each resonance.

GAMMA is an array in which the total width of each resonance is returned.

EONE is returned with the upper cutoff of the Nordheim calculation by resonance.

EPSIL is the lethargy mesh spacing for the Nordheim calculation of each resonance.

SIGOH is the peak value, σ_0, for each resonance.

XI is an array in which ξ is returned for each resonance.

MESH is an integer array in which the number of mesh points to be used in the Nordheim calculation is returned for each resonance.

AID is not used.

SPIN is an array of g_J for each resonance.

JPRINT is a print trigger flag (0/1 – yes/no) for information concerning the Nordheim resonance mesh parameters.

COMMON BLOCKS:

RSNNC

F2.5.6 ISRCH

CALLING SEQUENCE:

I = ISRCH (ID, MT, N, N)

FUNCTION:

ISRCH is used to locate a process identified by ID in a 1-D cross-section array MT dimensioned (M,N), where M is the number of groups plus 1 and N is the total number of processes. It returns the column number containing the process or a zero if the process cannot be found.

ARGUMENTS:

ID is the floating-point value of the identifier.

MT is the 1-D cross-section array.

M is the number of groups plus 1.

N is the number of processes in MT.

F2.5.7 LSRCH

CALLING SEQUENCE:

I = LSRCH (ID, I2, F3, MMT, IRES)

FUNCTION:

LSRCH is a logical function that is used to determine whether a nuclide with resonance parameters requires the allocation of arrays for the resonance calculation. Note that I and LSRCH are logical variables.

ARGUMENTS:

ID is the identifier of the nuclide.

I2 is the input array which specifies the nuclides from the master library (i.e., the 2$ array).

F3 is the input parameter array for resonance calculations (i.e., the 3* array).

MMT is the number of nuclides selected from the master library.

IRES is the number of blocks of input resonance data.

SUBROUTINES CALLED:

ISRCH

F2.5.8 MAXINT

CALLING SEQUENCE:

CALL MAXINT (AKT, TEMP, UKT, UL, UH, DU)

FUNCTION:

MAXINT is provided to allow calculating a group flux when the lower boundary of the group containing the resonance is less than 5 kT. In this case, the code calculates a flux integral as follows:

$$\phi_g = \int_{EL}^{5kT} dE\, M(E,T)dE + \int_{5kT}^{E_2} \frac{dE}{E},$$

which is added to the integral of the Nordheim Integral Treatment flux to get a value for the group. In the equation, EL is the lower energy of the group, M(E,T) is the Maxwellian flux, and E_2 is the lower cut-off of the Nordheim calculations. Both integrals above are determined analytically.

ARGUMENTS:

AKT is 5 kT expressed in eV.

TEMP is the temperature in Kelvin.

UKT is the lethargy corresponding to AKT.

UL is the lower lethargy boundary of the group.

UH is the higher lethargy boundary of the group.

DU is the flux value determined in this routine.

F2.5.9 MIXM

CALLING SEQUENCE:

CALL MIXM (A, L, C, IGM, IPM, I1, I2, N, IFTG, F)

FUNCTION:

MIXM is used to mix together transfer arrays that use the "magic-word" structure discussed in Sect. F2.3.8. It produces an expanded array that must subsequently be compressed using CMPS (see Sect. M2) for use in other situations.

ARGUMENTS:

A is the input transfer matrix which is to be added to C as follows:

$$C = C + F * A.$$

L is the length of the A array.

C is the expanded "summed" transfer matrix.

IGM is the number of neutron energy groups.

IPM is the number of gamma energy groups.

I1 is an offset that is added to the source group indices and is used for gamma groups when neutron and gamma data are combined into a single transfer matrix.

I2 is an offset that is added to the sink group indices and is used for gamma-gamma processes when neutron and gamma data are combined into a single transfer matrix.

N is an array containing the location of the "magic words" in the expanded transfer matrix, C.

IFTG is the first thermal neutron group.

F is a factor by which A is multiplied when it is added into C.

SUBROUTINES CALLED:

MGCWRD*

F2.5.10 MSTPRD

CALLING SEQUENCE:

CALL MSTPRD (X, CX, DE, LX, LY, LZ, SS, TP, UL, AID, AXS, ENG, EZR, GRD, IDE, MTT, MTX, MTY, MTZ, NLX, NLY, NLZ, NRL, NRX, NRY, NRZ, NTX, NTY, NTZ, RSA, RSN, RSS, CTTL, TEM, LENGTH, GAMN, GMGM, GFG, R, GAMMA, EONE, EPSIL, SIGOH, XI, MESH, ALPHA, TERM, IVAL, BVAL, SIGAZ, SIGSZ, F, AMU, SUB, DRI, SPIN, FACT, SEN, SEL, MSC, D, NNU)

FUNCTION:

MSTPRD is provided to access data from a master library and to provide control for the operations necessary to construct a file in AMPX working library format (see Sect. F2.3.8). The operations include calling RSNANC for resolved and unresolved resonance calculations, calling TERP1D to ensure that the set has values for total, absorption, capture, and elastic scattering cross sections, calling CRRCT to introduce resonance self-shielded values, calling SUMX to sum elastic and thermal P scattering matrices, calling FOLD to multiply yields by cross sections, calling RNORM to renormalize elastic scattering matrices, calling MIXM to mix together individual transfer matrices into a "total" transfer matrix, caling CMPS to compress an expanded "total" matrix, calling CSRT to correct for temperature-dependence of thermal scattering matrices, and calling SENSTY to produce a self-shielded AMPX master library. The output of MSTPRD is MMT sets of cross-section data on the working library.

ARGUMENTS:

X is a scratch array dimensioned by the number of gamma groups plus number of neutron groups. At one point, it is used to hold cross sections associated with gamma yields and later to store "magic word" positions in the expanded total transfer matrix, CTTL.

CX is an array set large enough to read any transfer matrix to be processed.

DE is an array dimensioned by the number of neutron groups into which the energy widths of the groups are placed in the resonance calculations.

MTX, LX, NLX, and NTX are arrays used to store neutron-scattering matrix directory data (see Sect. F2.3.8).

MTY, LY, NLY, and NTY are arrays used to store gamma-production matrix directory data.

MTZ, LZ, NLZ, and NTZ are arrays used to store gamma-scattering matrix directory data.

SS is an array used to store self-shielding factors for the Nordheim treatment. It is not used in NITAWL-S.

TP is the temperature array, which specifies thermal scattering matrix temperatures (4* Array).

UL is an array in which to read in neutron lethargy boundaries.

AID is a data array used to pass parameters to the resonance calculation.

AXS is not used.

ENG is an array used to store the neutron energy group boundaries.

EZR, GAMN, GMGM, GFG, R, and SPIN are arrays in which the resolved resonance parameters are circulated in the resonance routines. They correspond to E_0, Γ_n, Γ_γ, Γ_f, r, and g_J, respectively.

GRD is the input data block describing the resonance calculations (3* Array).

IDE is a 50-word array into which the nuclide directory data are read.

MTT is the input array which selects the nuclides to be read (2$ Array).

NRL is an array into which the starting records on direct access unit N9 of each P_ℓ matrix for a nuclide is stored.

NRX, NRY, NRZ are arrays used to read the directory for Bondarenko data.

RSA, RSN, RSS are arrays used by the Nordheim treatment and the unresolved treatment for storing the differences between self-shielded values for absorption, fission, and elastic scattering, and their infinite-dilution averages, respectively.

CTTL is an array into which data are "mixed" to form a total transfer matrix.

TEM is an array into which the thermal-scattering matrix temperatures are read.

LENGTH is an array for the compressed lengths of the P_ℓ total-transfer matrices.

EONE is an array in which are stored the starting energies for each resonance in the Nordheim calculation.

EPSIL is an array for the lethargy mesh (by resonance) for the Nordheim calculation.

SIGOH is an array for the peak cross sections, σ_0, of all resonances.

XI is an array for the ξ-values of all resonances.

MESH is an integer array for the number of mesh points to be taken for each resonance in the Nordheim calculation.

ALPHA is an array dimensioned by 3 for the α value of the fuel, moderator 1, and moderator 2, respectively.

TERM is an array dimensioned by 3 for storing the cumulative slowing down term for the fuel, moderator 1, and moderator 2, respectively.

IVAL is an array dimensioned by 3 for storing a mesh counter for the fuel, moderator 1, and moderator 2, respectively.

BVAL is an array dimensioned 1001*3 for storing contributions at each mesh in the Nordheim calculation for the absorber, moderator 1, and moderator 2, respectively.

SIGAZ and SIGSZ are arrays at which the point Doppler-broadened values are calculated for all points in the Nordheim mesh.

F is an array for the collision densities.

AMU is an array in which a quantity closely akin to the energy of each mesh point in the Nordheim calculation is stored.

SUB is an array in which the average flux in the lump at each mesh point in the Nordheim calculation is stored.

DRI is not used.

FACT is an array (called FACTOR in RSNANC) which is used to pass the abundance of the nuclide being calculated to the Nordheim treatment.

SEN and SEL are arrays into which the thermal and the epithermal elastic-scattering matrices are summed, in order to prepare for adjustment of 1-D cross sections.

MSC is the input array wherein the thermal process(es) is selected for nuclides having multiple kinds of thermal-scattering data (6$ Array).

D is the large container array allocated to NITAWL.

NNU is the total number of nuclides on the input master library.

SUBROUTINES CALLED:

CLEAR*, CMPS*, CRRCT, CXRT, FOLD, IO*, IO4*, JLL1*, MIXM, MWLIST*, PICKMT, PRTIME*, PRTID*, REED*, RITE*, RNORM, RSNANC, SENSTY, SUMS, SUMX, TERPID

COMMON BLOCKS:

COUNTR, RSNNC, DATA, DRTACS

F2.5.11 NDRVER

CALLING SEQUENCE:

CALL NDRVER (D, LLIM)

FUNCTION:

NDRVER serves as a control module for operations performed by NITAWL-II. In this routine, the second data block is read. The nuclide directories on up to three input cross-section libraries are read in order to determine maximum array sizes needed and, also, whether all nuclides requested are present. It sets up array pointers for practically all arrays used anywhere else in NITAWL-II. OPENDA is called to initialize direct access space on logical NT7. TAPERD is called to perform all operations requested for NITAWL-II. PRTIME is called to print elapsed time. CLOSDA is called to release the space for logical NT7 for use in other SCALE modules. RECTRY is called to ensure consistency of the nuclide directory on the working library output from NITAWL-II with actual data elsewhere on the library.

ARGUMENTS:

D is the large container array into which NITAWL-II builds its flexibly dimensioned arrays.

LLIM is the size of D (in 4-byte units).

SUBROUTINES CALLED:

CLOSDA, ERRO*, FIDAS*, ISRCH, OPENDA*, PRTIME*, QOREAD*, RECTRY*, TAPERD

COMMON BLOCKS:

EXECUT, DATA,COUNTR, RSNNC, DRTACS, BLKLNC

F2.5.12 NITAWL

CALLING SEQUENCE:

None (Main Program)

FUNCTION:

NITAWL is an alternative program to Q#$002 which is used to execute NITAWL-II in a non-SCALE environment, such as AMPX. It sets a parameter, IEXCT, to zero, thereby signaling that all input are made by card input. It calls SETUP, to initial and read the first data block. It calls ALOCAT to dynamically allocate core to NDRVER which controls the remainder of the NITAWL-II run.

SUBROUTINES CALLED:

SETUP, ALOCAT*, NDRVER (through ALOCAT)

COMMON BLOCKS:

EXECUT

F2.5.13 P0CYL

CALLING SEQUENCE:

CALL P0CYL (RI, RO)

FUNCTION:

P0CYL is used to calculate escape and transmission probabilities for annular cylindrical shells using the Bickley function formulation of Kier and Robba.[15]

ARGUMENTS:

RI is the value of $\bar{a}/\lambda$ at the inner shell.

RO is the value of $\bar{a}/\lambda$ at the outer shell.

F2.5.14 P0SPH

CALLING SEQUENCE:

CALL P0SPH (RI, RO)

FUNCTION:

P0SPH generates escape and transmission probabilities for spherical shells using the technique developed by Westfall.[14]

ARGUMENTS:

RI is the value of $\bar{a}/\lambda$ for the inner radius of the spherical shell.

RO is the value of $\bar{a}/\lambda$ for the outer radius of the spherical shell.

F2.5.15 PICKMT

CALLING SEQUENCE:

CALL PICKMT (CX, IGP, N1D, MT, X)

FUNCTION:

PICKMT is used to pick an array of values for a particular process from the AMPX 1-D array and return them in another array.

ARGUMENTS:

CX is the 1-D cross-section array from an AMPX library. It is dimensioned by number of processes times the number of groups plus 1.

IGP is the number of groups plus 1.

N1D is the number of processes in CX.

MT is the identifier of the process desired.

X is an array in which to return number of group values for process MT.

F2.5.16 RESOL

CALLING SEQUENCE:

CALL RESOL (UL, EZERO, GAMN, GMGM, GFG, GAMMA, EONE, EPSIL, SIGOH, MESH,ALPHA, TERM, IVAL, BVAL, SIGAZ, SIGSZ, F, AMU, SUB, RSA, RSN, RSS, DRI, SPIN, FACTOR, XI, AID, R)

FUNCTION:

RESOL is the principal routine for performing the Nordheim integral treatment. After initializing a few global variables, an outer loop is made over all resonances, where each resonance constitutes a separate and independent calculation. Within the loop, the first 100 or so statements are involved with the adjustment and determination of the α's of the fuel and two admixed moderators so as to cause the slowing-down integral meshes to fall on a common (Nordheim) mesh, while preserving the slowing-down power. The next segment of the outer loop is an approximately 50-line inner loop over the mesh to determine Doppler-broadened cross sections on the mesh which was predetermined in GRID. A second inner loop of approximately 100 lines is made over the mesh for the resonance, in order to determine collision densities and fluxes in the lump. Roughly half of this loop is devoted to a determination of the escape probability for the lump with the remaining half being used to evaluate the three slowing-down integrals necessary to evaluate the lump collision density. After the second inner loop a call is made to TRAPZ, which determines the averaged cross sections for absorption,

fission, and elastic scattering for the resonance. The call to TRAPZ occurs at the end of the outer loop over all resonances.

ARGUMENTS:

These arguments are as described for MSTPRD.

SUBROUTINES CALLED:

FSIGP*, P0CYL, P0SPH, SIMPSN, TRAPZ, VOGAM

COMMON BLOCKS:

DATA, RSNNC

F2.5.17 RNORM

CALLING SEQUENCE:

CALL RNORM (C, L, SGS, RSS, IGM, NR9, IO9)

PURPOSE:

RNORM is used to renormalize the elastic scattering matrix to agree with the self-shielded values.

ARGUMENTS:

C is the elastic transfer matrix in "magic-word" form.

L is the length of the elastic matrix.

SGS is an array that contains the original sums of the unshielded matrix by group.

RSS is an array of the self-shielded values.

IGM is the number of groups.

NR9 is the relative track pointer for direct-access unit IO9.

IO9 is the logical unit number for direct-access space onto which the self-shielded values are written.

SUBROUTINES CALLED:

MGCWRD*, RITE*

F2.5.18 RSNANC

CALLING SEQUENCE:

CALL RSNANC (ENG, UL, DE, SS, TTT, AID, EZERO, RSA, RSN, RSS, GAMN, GMGM, GFG, R, SPIN, FACTOR, GAMMA, EONE, EPSIL, SIGOH, XI, MESH, ALPHA, TERM, IVAL, BVAL, SIGAZ, SIGSZ, F, AMU, SUB, DRI)

FUNCTION:

RSNANC controls the resolved and unresolved resonance calculations in NITAWL-II. The first 150 lines are devoted to the resolved calculation, with the latter 100 lines for the unresolved. In the resolved part, after first initializing many values, the program extracts resonance parameters from the AMPX master library array and stuffs them into appropriate arrays. The program then edits resonance problem description data. GRID is called to determine parameters needed by the Nordheim calculation such as mesh attributes, σ_0, ξ, etc. RESOL is called to perform the resonance calculation and determine self-shielded values. The final part of RSNANC produces an edit of shielded values produced by the resonance calculation.

ARGUMENTS:

With only minor exceptions, the arrays to RSNANC have the same definitions as those discussed for MSTPRD. The exceptions are the following:

TTT is the resonance data array as read from the AMPX master library. (See Sect. F2.4, Record Type 4).

FACTOR is spelled FACT in MSTPRD.

SUBROUTINES CALLED:

ERRO*, GRID, RESOL

COMMON BLOCKS:

DATA, RSNNC

F2.5.19 SENSTY

CALLING SEQUENCE:

CALL SENSTY (CX, NRS, IDE, IGM, IPM, MTX, LX, NLX, NTX, MTY, LY, NLY, NTY, MTZ, LZ, NLZ, NTZ, N2DX, N2DY, N2DZ, IO9, NT9)

FUNCTION:

SENSTY is a subprogram used only in the case that it is desired to produce a self-shielded library written in the AMPX master library format, as opposed to the working library format normally output. The library is written on logical NT9 without resonance data (i.e., the resonance parameters and/or Bondarenko data are not carried; however, all partial transfer arrays are carried). In the case of gamma production arrays, the output will be in cross-section units only. Scattering matrices and 1-D data are passed in on direct-access scratch unit IO9. Only data for the temperature selected (4* Array) will be passed.

ARGUMENTS:

CX is space into which to read various arrays from IO9 in order to create NT9.

NRS is the track pointer for the first block of data to be read from IO9 for the nuclide.

IDE is a 50-word record in which the nuclide directory data will be created.

IGM is the number of neutron energy groups.

IPM is the number of gamma energy groups.

MTX, LX, NLX, NTX contain the scattering matrix directory of neutron cross sections.

MTY, LY, NLY, NTY contain the scattering matrix directory of gamma production data.

MTZ, LZ, NLZ, NTZ contain the scattering matrix directory of gamma cross sections.

N2DX is the number of neutron processes with scattering matrices.

N2DY is the number of gamma production processes with scattering matrices.

N2DZ is the number of gamma processes with scattering matrices.

IO9 is a scratch direct access unit containing cross sections for the nuclide.

NT9 is the logical unit of the device where the master library is to be written.

SUBROUTINES CALLED:

IO*, IO4*, REED*, YSCAN

COMMON BLOCKS:

DRTACS

F2.5.20 SETUP

CALLING SEQUENCE:

CALL SETUP

FUNCTION:

SETUP is provided to assign space for the initial data block, to read this data block and to open all input/output units prior to dynamically allocating space for the remainder of the NITAWL-II operations.

SUBROUTINES CALLED:

CLEAR*, INTIME*, MESAGE*, FIDAS*, QOREAD*

COMMON BLOCKS:

EXECUT, DATA, DRTACS, BLKLNC

F2.5.21 SIMPSN

CALLING SEQUENCE:

Value = SIMPSN (N, F, S1, S2, M, LMP)

FUNCTION:

SIMPSN is used to perform the recursive Simpson's integration described in Sect. F2.3.4.

ARGUMENTS:

N is the index of the panel value that will be subtracted when calculating the collision density at point M. (Note that SIMPSN is called separately for the absorber, and first and second moderators).

F is an array for the collision densities.

S1 is the "sum" of the points in F which will be multiplied by 4 in the Simpson's expression.

S2 is the "sum" of the points in F which will be multiplied by 2 in the Simpson's expression.

M is the point being calculated.

LMP is used to signal that S1 and S2 are to be initialized (LMP=0) or not initialized (LMP≠0).

F2.5.22 SUMS

CALLING SEQUENCE:

CALL SUMS (CX, L, X, IGM)

FUNCTION:

SUMS is used to zero an array, X, and to sum the "magic-word" transfer matrix, CX, into it.

ARGUMENTS:

CX is the "magic-word" transfer matrix.

L is the length of CX.

X is an array for the vector sums.

IGM is the number of energy groups.

SUBROUTINES CALLED:

MGCWRD*

F2.5.23 SUMX

CALLING SEQUENCE:

CALL SUMX (C, L, S)

FUNCTION:

SUMX is used to SUM a "magic-word" transfer matrix, C, into a vector, S. As opposed to SUMS, S is not initialized.

ARGUMENTS:

C is the "magic-word" transfer matrix.

L is the length of C.

S is an array for the vector sums.

SUBROUTINES CALLED:

MGCWRD*

F2.5.24 TAPERD

CALLING SEQUENCE:

CALL TAPERD (IDE, MSC, MTT, IDA, ENG, UL, DE, SS, AID, GRD, MARK, TP, GE, GU, MTX, LX, NLX, NTX, NRX, MTY, LY, NLY, NTY, NRY, MTZ, LZ, NLZ, NTZ, NRZ, NRL, X, TEM, LENGTH, CX, CTTL, AXS, EZERO, GAMN, GMGM, GFG, R, GAMMA, EONE, EPSIL, SIGOH, XI, MESH, ALPHA, TERM, IVAL, BVAL, SIGAZ, SIGSZ, F, AMU, SUB, DRI, SPIN, FACTOR, SEN, SEL, RSA, RSN, RSS, D)

FUNCTION:

TAPERD is a control module for reading information from the AMPX master and/or the two AMPX working/weighted libraries. The first ~150 lines are spent skipping over the header, nuclide directory, and energy boundary records on the three libraries and on making checks to ensure that all requested nuclides are present. At the same time, TAPERD writes the analagous records on the output working library and on the special\"self-shielded" master library, if this latter option is selected. The routine, MSTPRD, is called to read all data from the master library and to oversee the resonance calculations. The final ~75 lines are spent selecting data from the two input working libraries (if present) and on copying their data to the output working library.

ARGUMENTS:

Most of the arguments to TAPERD are for arrays that are passed to MSTPRD. Their definitions can be found in the discussion of this subprogram. The exceptions to this are the following:

MARK is an array dimensioned by the number of nuclides requested which is used to "mark"—MARK=1—which nuclides are found on one of the three input libraries.

GE is an array in which gamma energy boundaries are read.

GU is an array in which gamma lethargy boundaries are read.

X is a scratch array dimensioned by number of groups.

SUBROUTINES CALLED:

IO*, MSTPRD, MWLIST*, PRT1D*

COMMON BLOCKS:

COUNTR, DATA, RSNNC, DRTACS

F2.5.25 TERP1D

CALLING SEQUENCE:

CALL TERP1D (CX, N1D, IGP, NEW)

FUNCTION:

TERP1D is used to ensure that 1-D arrays exist for total (MT = 1), elastic (MT = 2), absorption (MT = 27), and capture (MT = 101). If they do not, it attempts to create them from the available data in such a manner as to ensure consistency.

ARGUMENTS:

CX is the 1-D cross-section array dimensioned (IGP, N1D).

N1D is the number of processes in CX.

IGP is the number of groups plus 1.

NEW is the number of arrays created in TERP1D.

SUBROUTINES CALLED:

CLEAR*

F2.5.26 TRAPZ

CALLING SEQUENCE:

CALL TRAPZ (MESH, WING, S, FF, FL, IFTG, SETE, E1, EPS, UL, SUB, SIGA, SIGS, RSA, RSN, RSS, GFG, TABS, TFIS, FACT, VF, UHI, ULO, SP, TEMP, AKT, IGM)

FUNCTION:

TRAPZ is used to determine the average cross sections by group for each resolved resonance. Values are calculated for absorption, fission, and elastic scattering. The procedure, which includes provisions for a "cell" weighting, is described in Sect. F2.3.5.

ARGUMENTS:

MESH is the number of mesh points taken in the resonance.

WING is not used.

S is not used.

FF is not used.

FL is not used.

IFTG is the last group that should receive a resonance treatment (typically the last group).

SETE is the energy of the lethargy zero (normally 10^7 eV).

E1 is the upper boundary of the Nordheim calculation.

EPS is the Nordheim lethargy mesh size.

UL is an array of lethargy boundaries for all groups.

SUB is an array of fluxes determined by the Nordheim treatment.

SIGA is an array for the Doppler-broadened point absorption cross sections.

SIGS is an array for the Doppler-broadened point scattering cross sections.

RSA is an array for the group-averaged absorption cross sections.

RSN is an array for the group-averaged fission cross sections.

RSS is an array for the group-averaged elastic-scattering cross sections.

GFG is the ratio of $\Gamma_f/(\Gamma_f+\Gamma_\gamma)$ for the resonance.

TABS is where the total absorption resonance integral is accumulated.

TFIS is where the total fission resonance integral is accumulated.

FACT is the abundance of the nuclide whose resonance is being calculated.

VF is the volume fraction of the lump in the fuel cell.

UHI is the upper lethargy boundary for the resolved resonance region.

UHO is the lower lethargy boundary for the resolved resonance region.

SP is the potential scattering cross section.

TEMP is the temperature in the lump.

AKT is the upper energy cutoff for a Maxwellian flux shape at low energies.

IGM is the number of energy groups.

SUBROUTINES CALLED:

MAXINT

F2.5.27 VOGAM

CALLING SEQUENCE:

CALL VOGAM (X631, X632, PSI, CHI)

FUNCTION:

VOGAM is used to determine ψ and X for use in Doppler broadening of resonances.

ARGUMENTS:

X631 is $2.0\ (E-E_0)/\Gamma$.

X632 is $\frac{4.0}{\Gamma}\sqrt{kTE_0/A}$.

PSI is the returned value of ψ.

CHI is the returned value of X.

F2.5.28 YSCAN

CALLING SEQUENCE:

CALL YSCAN (X, LN, LW, IGM)

FUNCTION:

YSCAN is used to determine the last "really used" position in a "magic-word" transfer matrix. In this case, it senses the negative magic-word which denotes the end of the matrix.

ARGUMENTS:

X is the cross-section array.

LN is the total length of the array.

LW is the "usable" length of the array.

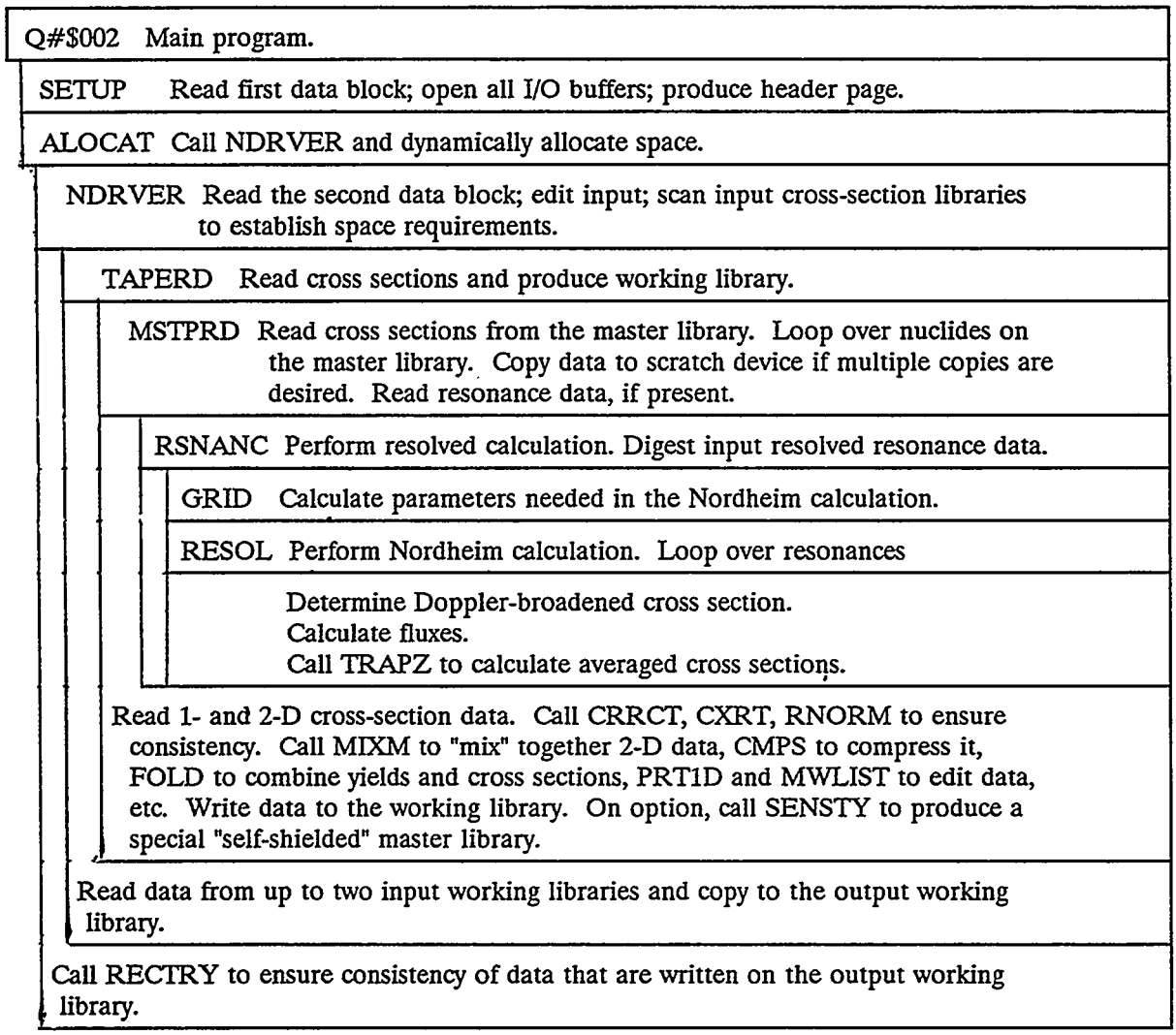
IGM is the number of neutron energy groups.

SUBROUTINES CALLED:

MGCWRD*

F2.6 PROGRAM STRUCTURE INFORMATION FLOW

The program flow of NITAWL-II is reasonably simple as shown in the following chart:



F2.7 INPUT SPECIFICATIONS

The following is a description of input requirements and input-output device requirements.

F2.7.1 INPUT PARAMETERS

All card input to NITAWL-II uses FIDO-type input (see Sect. M10). The number of items to be input in an array is shown in brackets, while default values are given in parentheses.

Data Block 1

–1$ Core Assignment [1]

1. LIMIT – the number of words allocated to the container arary for NITAWL-II. (200000)

0$ Logical Assignments [9]. This array is input only if a user needs to modify default values.

1. N1 – Input Master Cross-Section Interface (1)
2. N2 – Input Working/Weighted Cross-Section Interface (2)
3. N3 – Input Working/Weighted Cross-Section Interface (3)
4. N4 – Working Cross-Section Interface produced by NITAWL-II (4)
5. N5 – Scratch (18)
6. N6 – Scratch (19)
7. N7 – Random Access Scratch (9)
8. N8 – Not Used (15)
9. N9 – Master Sensitivity Interface produced by NITAWL-II (20)

1$ Integer Parameters [12]

1. MSCM – Number of mesh intervals per resonance. (500)
2. MMT – Number of nuclides to read from the master cross-section library mounted on N1. Resonance calculations can be made with "resonance" nuclides from a master library, but not from a working/weighted library. (0)
3. MWT – Number of nuclides to read from the working/weighted library on logical N2. (0)
4. MXT – Number of nuclides to read from the working/weighted library on logical N3. (0)

5. MCR – Sensitivity output trigger (0)

   = 0, do not produce master sensitivity library
   > 0, produce master sensitivity library

   Note: The master sensitivity library will contain only nuclides selected from the master cross-section library on logical N1.

6. MXX – Not Used (0)

7. MS – Not Used (0)

8. IRES – Number of resonance calculations to be performed. (0)
   Resonance data are required in the 3* array discussed below.

9. IQM – Highest resonance ℓ-value for which a self-shielding calculation will be performed.

10. IPM – Not Used (0)

11. IPP – Output option trigger (0)
    0 – no cross-section edits
    1 – edit reaction cross sections
    >1 – edit reaction cross sections and transfer arrays through order IPP-2

12. IFG – Not Used (0)

T Terminate this data block.

Data Block 2

2$ Identification Numbers of Nuclides to be Placed on the Working Library
[MMT+MWT+MXT]

NITAWL-II can combine data from three sources to make a working library on logical unit N4. This working library contains only those nuclides selected and is intended for use by another SCALE module such as XSDRNPM/S or KENO-V/S to solve a particular problem. The nuclide identifications are input in the order:

1. MMT identifications for nuclides from the master library on N1.

2. MWT identifications for nuclides from the working/weighted library on N2.

3. MXT identifications for nuclides from the working/weighted library on N3.

Within each group, the identifications can be in any order.

A facility is provided for creating duplicate sets for a particular nuclide. For example, a resonance nuclide might occur in different compositions, thereby requiring different resonance calculations. To create a new set, place a unique negative number in the identification string after the nuclide's identification which is to be

duplicated. As many sets as needed can be had, merely by stringing out negative numbers. All subsequent references to the new sets of data should use a positive identification. The values MMT, MWT, and MXT must be increased to reflect the inclusion of these sets.

3* Resonance Data [IRES*15] (IRES>0)

For each resonance calculation, 15 items are required. These blocks of data are placed, one set after the other, in any order in the 3* array. Note that only one 3* array is input. Resonance calculations can only be performed on resonance nuclides from a master library. The 15 items are:

1. Nuclide's identification number.

2. Temperature (K).

3. Geometry for Nordheim treatment
   0 – homogeneous,
   1 – slab,
   2 – cylindrical,
   3 – spherical.

4. Absorber lump dimension in centimeters (i.e., the thickness of the slab or outer radius of the sphere or cylinder). A zero is used for the homogeneous case.

5. Dancoff correction factor. This factor corrects for shadowing effects due to the presence of other absorber lumps (e.g., fuel elements) in the neighborhood of the lump being calculated. It is zero for the homogeneous and the one lump case.

6. a_i, the inner radius of the spherical or cylindrical shell, if a "shell" geometry is required. (Note that a value of zero specifies a solid sphere or cylinder. If the inner region **does not** contain a light-mass moderating material, the absorber should be treated as a solid.) (0.0)

7. N_a, absorber number density in the lump.

8. Treatment of absorber's contribution to the collision density.
   1 – Nordheim integral method
   2 – narrow resonance approximation
   3 – infinite mass approximation

9. Atomic mass of the first moderator in the lump. The resonance routines have provisions for treating two moderators.

10. σ_{s1}, scattering cross section for the first moderator in per absorber atom units.

$$\sigma_{s1} = N_1 \, \sigma_s \text{ (moderator 1)}/N_a ,$$

where N_1 is the number density of the first moderator.

11. Treatment of the first moderator's contribution to the collision density.
    0 – no first moderator
    1 – Nordheim's integral method
    2 – asymptotic approximation

12. Atomic mass of the second moderator in the lump.

13. σ_{s2}, scattering cross section for the second moderator in per absorber atom units.

14. Treatment of the second moderator's contribution to the collision density.
    0 – no second moderator
    1 – Nordheim's integral method
    2 – asymptotic approximation

15. Volume fraction of the absorber lump in the cell. This parameter is used for "cell averaging" the resonance cross sections, and would normally be 1.0 (see Sect. F2.4).

4* Thermal-Scattering Kernel Temperatures for Nuclides Selected (K) [MMT]

Scattering kernels are sometimes provided at several temperatures for a nuclide. NITAWL-II will pick the one closest to the temperature input in this array. This array has no effect for sets of data with zero or one thermal kernel.

6$ MT number of the Incoherent Thermal-Scattering Kernel [MMT]

These allow selecting a thermal-scattering kernel with an MT (identifying) number other than the default (1007).

T Terminate this data block.

F2.7.1.1 Abbreviated Input Description

Users who become familiar with the values required by NITAWL-II will become dissatisfied with having to use a detailed input description. The description that follows is intended to serve as a "skeleton" guide for these users:

Data Block 1

0$ Logical Assignments (9)
1. MMTI – Master In (1)
2. MWTI – Working In (2)
3. MXTI – Weighted In (3)
4. MTWTO – Working Out (4)
5. MSC1 – Scratch (18)
6. MSC2 – Scratch (19)
7. NDA – Direct Access (9)
8. N8 – (0)
9. NSN – Sensitivity (20)

1$ Integer Parameters [12]
1. NPTS– pts per res (500)
2. NMT – number from master
3. NWT – number from working
4. NXT – number from weighted
5. MCR – sensitivity trigger
6. MXX – 0
7. MS – 0
8. NRES – number res calc
9. IQM – 0
10. IPM – 0
11. IPP – cross-section edit option
12. IFG – 0

T Terminate Block 1.

Data Block 2

2$$ Identifiers of Nuclides (NMT+NWT+NXT)

3** Resonance Calculation Data (15*NRES)
1. Nuclide ID
2. T
3. geometry (0, 1, 2, 3/hom, slab, cyl, sphere)
4. outer dimension
5. Dancoff
6. inner dimension
7. N_a
8. 1, 2, 3/Nordheim, NR, IM
9. M_1
10. σ_{s1}
11. 0, 1, 2/none, Nordheim, NR
12. M_2
13. σ_{s2}
14. 0, 1, 2/none, Nordheim, NR
15. VF of lump in cell

4** Thermal Kernel Temperatures

6$$ MT's for Incoherent Matrices

T Terminate Block 2

F2.7.2 INPUT/OUTPUT ASSIGNMENTS

NITAWL-II typically requires the following input-output devices during an execution.

Logical Number	Purpose
NT1 (1)	Master Cross-Section Library
NT2 (2)	Previously Prepared Working/Weighted Library
NT3 (3)	Previously Prepared Working/Weighted Library
NT4 (4)	New Working Library
NT5 (18)	Scratch Unit
NT6 (19)	Scratch Unit
NT7 (9)	Random-Access Scratch Unit
NT9 (20)	Produced Master Sensitivity Library
5	Card Input (when run outside of SCALE)
6	Printed Output
97	Binary Input Unit (when run in the SCALE system)

F2.8 SAMPLE PROBLEM

A sample problem representing a low-enriched UO_2 fuel pin has been included to lillustrate using NITAWL-II. The fuel is 2.35% enriched and clad with zirconium. The Dancoff factor corresponds to a pitch of 1.27 cm.

F2.8.1 SAMPLE PROBLEM INPUT

Figure F2.8.1 shows the input for the sample problem. The 0$ Array specifies reading a master libary on unit 82. The 1$ Array specifies selecting five nuclides from the master library, and doing two resonance calculations. The 2$ Array lists the five nuclides requested from the master library: hydrogen (1001), oxygen (8016), zirconium (40000), U-235 (92235), and U-238 (92238). The 3* Array specifies the data needed to do resonance calculations for U-235 and U-238. The calculations are specified as being at room temperature (293 K) for cylinders with a radius of 0.4115 cm. The 4* Array specifies selecting the thermal scattering kernel closest to 293 K for any nuclide having multiple-scattering kernels.

```
0$$ 82 E 1$$ 0 5 A8 2 A11 0 E 1T
2$$ 1001 8016 40000 92235 92238 3**
92235 293 2 .4115 .251 0.0 4.8853-4 1 15.994 315.2 1 238.125 340.5 1 1
92238 293 2 .4115 .251 0.0 2.0044-2 1 15.994 7.683 1 235.117 0.256 1 1
4** F293 2T
```

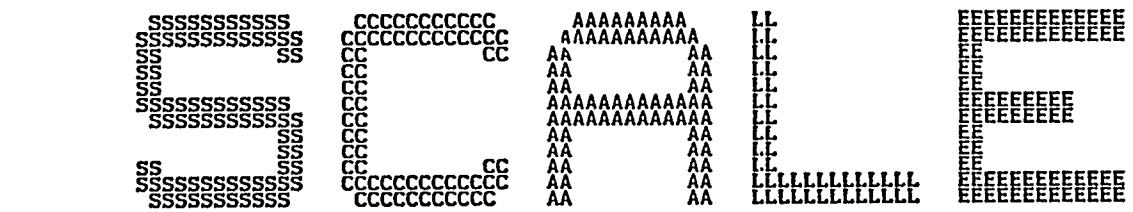
Figure F2.8.1 Sample problem input

F2.8.2 SAMPLE PROBLEM OUTPUT

Figure F2.8.2 shows the output for the NITAWL-II sample problem. The first page is a separator page listing the code, job name, date, and time of day the sample problem was executed. The second page lists the arrays read in the first data bock, then prints back the 1$ Array. The number of words in the storage array is then listed. Next comes the arrays read in the second data block. A table of information read from the master library is printed followed by a line giving the requirements of the random access scratch unit. The title of the master library is then printed, followed by a table of the nuclides selected from the master. The next page contains a list of the title records of each nuclide as it is found on the master library. After the hydrogen record, a line giving the temperature of the thermal scattering kernel actually selected is printed. After the U-235 and U-238 title records, a table giving the data used in the resonance calculation is printed, followed by a table giving the resonance absorption, fission, and scattering cross sections by group. This table includes only the cross section calculated in the resonance calculation and excludes any background contribution. Also, the resonance scattering does not have the potential scattering cross section added in. After each resonance calculation, the elapsed time to that point is printed. After all the nuclides have been copied from the master library, the total elapsed time is printed. The next page contains the table of contents of the working library produced by NITAWL-II.

```
MODULE NITAWL   WILL BE CALLED  TIME OF DAY 11.18.40  DATE 92.136
  0$$ 82 E  1$$ 0 5 A8 2 A11 0 E  1T
  2$$ 1001 8016 40000 92235 92238  3**
  92235 293 2 .4115 .251 3153. 4.8853-4 1 15.994 315.2 1 238.125 340.5 1 1
  92238 293 2 .4115 .251 76.86 2.0044-2 1 15.994 7.683 1 235.117 0.256 1 1
  4** F293 2T
  END
MODULE NITAWL   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED    17.98 (SECONDS). I/O'S USED       0.
```

Figure F2.8.2 Sample problem output




```
PROGRAM VERIFICATION INFORMATION
CODE SYSTEM:  SCALE . VERSION:  4.1

        PROGRAM:  NITAWL
  CREATION DATE:  91.350
        LIBRARY:  E.TZA27286.NEAD.PGMS77

 PRODUCTION CODE:  NITAWL
       REVISION:  1.6
        JOBNAME:  USMNITAL
DATE OF EXECUTION:  05/15/92
TIME OF EXECUTION:  11.18.45
```

Figure F2.8.2 (continued)

```
    0$ ARRAY       9 ENTRIES READ
    1$ ARRAY      12 ENTRIES READ
    1T
SELECT   5 NUCLIDES FROM THE MASTER  LIBRARY ON LOGICAL 82
         0 NUCLIDES FROM THE WORKING LIBRARY ON LOGICAL  2
         0 NUCLIDES FROM THE WORKING LIBRARY ON LOGICAL  3
           TO CREATE THE NEW WORKING LIBRARY ON LOGICAL  4

         2 RESONANCE CALCULATIONS HAVE BEEN REQUESTED
         0 OUTPUT OPTION FOR AMPX FORMATTED CROSS SECTION DATA
THE STORAGE ALLOCATED FOR THIS CASE IS 200000 WORDS
    2$ ARRAY       5 ENTRIES READ
    3* ARRAY      30 ENTRIES READ
    4* ARRAY       5 ENTRIES READ
    2T
 GENERAL INFORMATION CONCERNING CROSS SECTION LIBRARY
   TAPE IDENTIFICATION NUMBER                4027000
   NUMBER OF NUCLIDES ON TAPE                     83
   NUMBER OF NEUTRON ENERGY GROUPS                27
   FIRST THERMAL NEUTRON ENERGY GROUP             15
   NUMBER OF GAMMA ENERGY GROUPS                   0
   DIRECT ACCESS UNIT NUMBER  9 REQUIRES 117 BLOCKS OF LENGTH  1484 WORDS

 XSDRN TAPE4027000          SCALE 4 - 27 NEUTRON GROUP CRITICALITY SAFETY LIBRARY
                              BASED ON ENDF-B VERSION 4 DATA
                                COMPILED FOR NRC       1/27/89
                                  LAST UPDATED        10/12/89
                                    L.M.PETRIE        ORNL

 NUCLIDES FROM XSDRN TAPE
    1     HYDROGEN       ENDF/B-IV MAT 1269/THRM1002    UPDATED 10/12/89          1001
    2     OXYGEN-16      ENDF/B-IV MAT 1276             UPDATED 10/12/89          8016
    3     ZIRCONIUM      ENDF/B-IV MAT 7141             UPDATED 10/12/89         40000
    4     URANIUM-235    ENDF/B-IV MAT 1261             UPDATED 10/12/89         92235
    5     URANIUM-238    ENDF/B-IV MAT 1262             UPDATED 10/12/89         92238

 HYDROGEN        ENDF/B-IV MAT 1269/THRM1002  UPDATED 10/12/89
                       THERMAL SCATTERING MATRIX NUMBER  1 AT A TEMPERATURE OF   1001   TEMPERATURE=  293.00
                                                                                  293.00 WAS SELECTED.
 OXYGEN-16       ENDF/B-IV MAT 1276           UPDATED 10/12/89          8016    TEMPERATURE=  293.00
 ZIRCONIUM       ENDF/B-IV MAT 7141           UPDATED 10/12/89         40000    TEMPERATURE=  293.00
 URANIUM-235     ENDF/B-IV MAT 1261           UPDATED 10/12/89         92235    TEMPERATURE=  293.00
THE INNER RADIUS WAS SPECIFIED AS  3.15300E+03 WHICH IS GREATER THAN A-BAR. IT HAS BEEN SET TO 0.0
RESONANCE DATA FOR THIS NUCLIDE
MASS NUMBER (A)          =   233.025          TEMPERATURE(KELVIN)       =   293.000
POTENTIAL SCATTER SIGMA  =    11.500          LUMPED NUCLEAR DENSITY    = 4.8852991E-04
SPIN FACTOR (G)          = 15171.098          LUMP DIMENSION (A-BAR)    = 4.1149998E-01
INNER RADIUS             = 0.0000000E+00      DANCOFF CORRECTION (C)    = 2.5099999E-01
THE ABSORBER WILL BE TREATED BY THE NORDHEIM INTEGRAL METHOD.
MASS OF MODERATOR-1    =    15.994           SIGMA(PER ABSORBER ATOM)= 3.1519995E+02
MODERATOR-1 WILL BE TREATED BY THE NORDHEIM INTEGRAL METHOD.
MASS OF MODERATOR-2    =   238.125           SIGMA(PER ABSORBER ATOM)= 3.4050000E+02
MODERATOR-2 WILL BE TREATED BY THE NORDHEIM INTEGRAL METHOD.
THIS RESONANCE MATERIAL WILL BE TREATED AS A 2-DIMENSIONAL OBJECT.
VOLUME FRACTION OF LUMP IN CELL USED TO ACCOUNT FOR SPATIAL SELF-SHIELDING=1.00000
GROUP        RES ABS          RES FISS         RES SCAT
  12     -2.317591E+00    -1.423825E+00    -5.766904E-02
  13     -7.684970E+00    -3.765014E+00    -1.706647E-01
  14     -5.613071E+00    -3.349269E+00    -3.896813E-02
EXCESS RESONANCE INTEGRALS
```

Figure F2.8.2 (continued)

```
                    RESOLVED
ABSORPTION        2.08548E+02
FISSION           1.24378E+02

  ELAPSED TIME    0.12 MIN.

 URANIUM-238    ENDF/B-IV MAT 1262          UPDATED 10/12/89          92238     TEMPERATURE=    293.00
THE INNER RADIUS WAS SPECIFIED AS  7.68600E+01 WHICH IS GREATER THAN A-BAR. IT HAS BEEN SET TO 0.0
RESONANCE DATA FOR THIS NUCLIDE
MASS NUMBER (A)          =   236.006          TEMPERATURE(KELVIN)       =   293.000
POTENTIAL SCATTER SIGMA  =    10.599          LUMPED NUCLEAR DENSITY    = 2.0043999E-02
SPIN FACTOR (G)          =   656.527          LUMP DIMENSION (A-BAR)    = 4.1149998E-01
INNER RADIUS             = 0.0000000E+00      DANCOFF CORRECTION (C)    = 2.5099999E-01
THE ABSORBER WILL BE TREATED BY THE NORDHEIM INTEGRAL METHOD.
MASS OF MODERATOR-1    =    15.994           SIGMA(PER ABSORBER ATOM)= 7.6829996E+00
MODERATOR-1 WILL BE TREATED BY THE NORDHEIM INTEGRAL METHOD.
MASS OF MODERATOR-2    =   235.117           SIGMA(PER ABSORBER ATOM)= 2.5599998E-01
MODERATOR-2 WILL BE TREATED BY THE NORDHEIM INTEGRAL METHOD.
THIS RESONANCE MATERIAL WILL BE TREATED AS A 2-DIMENSIONAL OBJECT.
VOLUME FRACTION OF LUMP IN CELL USED TO ACCOUNT FOR SPATIAL SELF-SHIELDING=1.00000
GROUP        RES ABS          RES FISS         RES SCAT
  9      -4.612604E-02    0.000000E+00    -4.569043E-01
 10      -1.135619E+00   -2.311320E-05    -6.879468E+00
 11      -9.871305E+00    0.000000E+00    -2.709233E+01
 12      -4.290237E+01    0.000000E+00    -4.988403E+01
 13      -5.369963E+01    0.000000E+00    -1.762585E+01
 14      -1.040034E+02    0.000000E+00    -6.036744E+00
EXCESS RESONANCE INTEGRALS
                    RESOLVED
ABSORPTION        1.89507E+01
FISSION           4.94416E-04

  ELAPSED TIME    0.28 MIN.

  ELAPSED TIME    0.29 MIN.
```

Figure F2.8.2 (continued)

```
THIS XSDRN WORKING TAPE WAS CREATED 05/15/92 AT 11.19.16
THE TITLE OF THE PARENT CASE IS AS FOLLOWS
SCALE 4 - 27 NEUTRON GROUP CRITICALITY SAFETY LIBRARY
  BASED ON ENDF-B VERSION 4 DATA
    COMPILED FOR NRC       1/27/89
    TAPE ID                      4027000          NUMBER OF NUCLIDES                5
    NUMBER OF NEUTRON GROUPS          27          NUMBER OF GAMMA GROUPS            0
    FIRST THERMAL GROUP               15          LOGICAL UNIT                      4
                                  TABLE OF CONTENTS
   HYDROGEN        ENDF/B-IV MAT 1269/THRM1002    UPDATED 10/12/89          ID     1001
   OXYGEN-16       ENDF/B-IV MAT 1276             UPDATED 10/12/89          ID     8016
   ZIRCONIUM       ENDF/B-IV MAT 7141             UPDATED 10/12/89          ID    40000
   URANIUM-235     ENDF/B-IV MAT 1261             UPDATED 10/12/89          ID    92235
   URANIUM-238     ENDF/B-IV MAT 1262             UPDATED 10/12/89          ID    92238

    TAPE COPY USED      0 I/O'S, AND TOOK     0.32 SECONDS
```

Figure F2.8.2 (continued)

F2.9 ERROR MESSAGES

NITAWL produces error messages in some cases where it detects an improper request has been made or when inadequate core has been provided for the run. In most cases, these are self-explanatory. The listing below will attempt to explicitly describe the "problem." The messages are blocked according to the subroutine in which they are issued.

MSTPRD

THE NEUTRON CROSS SECTIONS CANNOT BE FOUND TO CONVERT THE YIELDS FOR ENDF MT = mmmm

On a master library, photon yields are carried in "yield" units, wherever possible. These units are expected to be combined with a reaction cross section prior to placing them in a working library. The most obvious way to get this error would be to use a library directly out of LAPHNGAS, which does not produce group-averaged neutron values. A neutron library such as XLACS should be "coupled" with the LAPHNGAS library.

THE MASTER LIBRARY IS NOT MARKED AS HAVING RESONANCE DATA CONSISTENT WITH NITAWL2

This message is produced whenever the AMPX master library is one of the earlier versions that referenced the resonance calculation to "background" data. A code called CORECTOL is available to convert the older formats to the newer ones. CORECTOL is a member of the AMPX system.

NDRVER

STOR nnnnnn

The module has insufficient core to execute the problem. One must allocate at least nnnnnn words. Increase the number of words allocated in the -1$ array.

PARAMETERS ON THE TAPE ON UNIT *lll* DO NOT MATCH THE OLD SET

.
.
.
.

The user has requested using cross-section data from two or more libraries that have different neutron or energy group structures. The user must ensure that the input master, working and/or weighted libraries are consistent.

NITAWL

INSUFFICIENT STORAGE IN NITAWL

This error indicates that the core region assigned to NITAWL will not accommodate the working array size requested. Either assign more core and/or increase the number of words requested by the parameter in the -1$ array.

RESOL

A LUMP VOLUME FRACTION OF 0.0 MAKES NO SENSE

The fifteenth parameter in the resonance calculational data is the volume fraction of the fuel lump in the cell. It is not physical to say that the fraction is zero. This parameter is only used in the determination of the "cell-averaged" values, and a zero will work, though the user should carefully examine the defining equations which will look like using the real flux in the $\int \sigma \phi$ term, divided by Δu_g in the denominator.

THERE HAS BEEN A FORMAT MODIFICATION TO RESONANCE PARAMETER.....SEE THE COMET EXPERT.....

As part of the data associated with ENDF/B resonance parameters, there is an energy range over which the parameters should be used. This range is needed to help the Nordheim calculation to be made outside this range. A module called COMET can be used to introduce the proper range.

RSNANC

AN OPTION NUMBER IS INCORRECT, THE INPUT IS AS FOLLOWS:

GEOMETRY= ABSORBER=
MODERATOR1= MODERATOR2=

In the resonance calculational input data, the geometry option should be between 0 and 3, the absorber calculational option should be 1, 2, or 3, while the moderator calculational options should be 0, 1, or 2.

GEOMETRY HAS BEEN SET TO HOMOGENEOUS AS LBAR IS 0.0

A user has selected a "finite" geometry (slab, cylinder, or sphere) and input $\bar{a}$ as zero.

THE INNER RADIUS WAS SPECIFIED AS A VALUE WHICH IS GREATER THAN A-BAR. IT HAS BEEN SET TO 0.0

Self explanatory. The user may want to redo the input and resubmit the problem.

TAPERD

FOLLOWING NUCLIDES WERE NOT FOUND

The user has requested nuclides that are not on the input libraries.

POSSIBLE TROUBLE—YOU ASKED FOR nnn NUCLIDES BUT THIS CODE ONLY FOUND mmm

This message is given in conjunction with the previous one.

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Computing Applications Division

XSDRNPM: A ONE-DIMENSIONAL DISCRETE-ORDINATES CODE FOR TRANSPORT ANALYSIS

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ABSTRACT

XSDRNPM is a discrete-ordinates code that solves the one-dimensional Boltzmann equation in slab, cylindrical, or spherical coordinates. Alternatively, the user can select P_1 diffusion theory, infinite medium theory, or B_n theory. A variety of calculational types are available, including fixed source, eigenvalue, or "search" calculations. In SCALE, XSDRNPM is used for several purposes: eigenvalue (k-effective) determination, cross-section collapsing, shielding analysis, and for producing bias factors for use in Monte Carlo shielding calculations.

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F3.1 INTRODUCTION

XSDRNPM is a one-dimensional (1-D) discrete-ordinates transport code and is the latest in a series of codes in the XSDRN[1] family. As such, it contains several unique characteristics, as will be detailed in this report, though a large portion of the theoretical bases and intended uses of the program are the same for all versions.

F3.1.1 FUNCTIONS PERFORMED

The function of XSDRNPM is twofold: (1) perform a 1-D discrete-ordinates calculation in slab, cylindrical, or spherical geometry (optionally, a 1-D diffusion theory or infinite medium B_n calculation can be made), and (2) use the fluxes determined from its spectral calculation to collapse input cross sections and write these into one of several formats.

A great deal of flexibility is allowed in describing a problem for XSDRNPM. The number of spatial intervals, the number of energy groups, the number of nuclides, the quadrature order, the order of fits to the angular variation in basic cross sections are all arbitrary and are limited only by computer and monetary resources.

The flux calculation can be performed according to several options, including fixed source calculations, k-calculations, and dimension search calculations.

A variety of weighting options are allowed, including zone, cell, or a special "vein" weighting option which is described herein.

F3.1.2 BACKGROUND ON XSDRNPM

Development of the XSDRN[1] program started in the mid-1960s. The goal was to develop a program that would combine features from the GAM-II,[2] ANISN,[3] and THERMOS[4] programs in a more unified and general way than would be possible if one simply elected to use these codes individually.

The salient features to be retained from the programs were as follows:

GAM-II	The Nordheim Integral Treatment was desired for resonance self-shielding; the generality of including cross sections for an arbitrary number of processes, along with the provisions for truncating zero or impossible transfers in the scattering matrices, was also a requirement.
ANISN	One-dimensional discrete-ordinates or diffusion theory or infinite-medium theory was to be available to generate a spectrum for cross-section collapsing.
THERMOS	The ability to perform detailed 1-D spectral calculations, including upscatter effects, was required for the thermal region.

The whole code was required to be dynamically dimensioned to allow calculations for arbitrary group structures, spatial structures, angular quadratures, etc.

The XSDRN program that embodied these features was released in 1969.

In the early 1970s, the Defense Nuclear Agency (DNA) initiated support for the AMPX system, which was to be a total cross-section generation system capable of performing all tasks necessary to take basic neutron and gamma-ray cross-section data and process these data into the proper form needed for weapons effects calculations. Since XSDRN already encompassed many of the features needed, it was selected as a basis for modules in the new system. In this case, experience developed in the original construction of XSDRN served to suggest that a more modular approach would have been better with independent tasks being done in separate, smaller, easier-to-manage programs. Therefore, the code was split into NITAWL-II (for resonance self-shielding and some basic cross-section data manipulation; see Sect. F2) and XSDRNPM (for spectral calculations and cross-section collapsing). In retrospect, if the AMPX development were initiated today, XSDRN would have been split even further, into perhaps as many as six or seven programs.

The XSDRNPM module differs from XSDRN in several respects:

- It will perform coupled neutron-gamma calculations.
- It allows any mixture to be represented to an arbitrary order of anisotropic representation, whereas XSDRN only allowed through order 3.
- It will perform an adjoint calculation, whereas the option was never provided in XSDRN.
- It is considerably more efficient in the manner in which data storage is used and, hence, will run much larger problems in less core storage.
- It employs improved thermal flux scaling techniques for better problem convergence.
- Input specifications have been reordered, and more defaults have been provided to make the use of this module easier.
- It will calculate S_n constants for any order for any of the three 1-D geometries available.
- Mixture-dependent fission spectra are calculated and used in XSDRNPM, which takes into account all fissionable nuclides in a problem.

AMPX was released in 1976, about the same time as the U.S. Nuclear Regulatory Commission (NRC) support for the SCALE system was initiated. Although separate versions of XSDRNPM were initially maintained for AMPX and SCALE, in recent years the same version is used for the two systems.

F3.1.3 APPLICATIONS IN SCALE

XSDRNPM is used in several places in SCALE. In SAS1 (Sect. S1), XSDOSE uses fluxes from a 1-D shielding calculation to determine a dose rate. In SAS2 (Sect. S2), XSDRNPM is used in a cell-weighting procedure to produce one-group cross-section values for ORIGEN (Sect. F7) and to perform a 1-D shielding calculation to generate fluxes for XSDOSE as in SAS1. In SAS3 (Sect. S3), XSDRNPM is again used for cell weighting. In the SAS4 path, an adjoint XSDRNPM calculation will be performed as part of the procedure to produce Monte Carlo biasing factors. Within the CSAS control module, XSDRNPM is used in the sequences to perform eigenvalue calculations and cell weighting of cross sections.

F3.1.4 NOTES ON THE USE OF VARIOUS SPECTRAL CALCULATIONAL OPTIONS

As noted earlier, four options are available in XSDRNPM for calculating fluxes, k-effectives, etc.:

1. S_n theory,
2. diffusion theory,
3. infinite medium theory, and
4. B_n theory.

However, XSDRNPM is primarily an S_n code. The latter three options are provided for reasons of completeness and are not nearly as optimized as they would be in other codes for which these are the primary spectral calculation options.

Without a very detailed calculational study, it is perhaps impossible to be able to quantify the degree of adequacy or inadequacy of any of these methods for performing a particular problem. However, some general comments can be made which may provide some guidance with their selection.

First, S_n theory is the most correct of the options and will solve a larger class of problems. Unfortunately, it is also the most complicated and time-consuming of the four. There are problems, however, for which it (or some alternative method based on a solution of the Boltzmann equation) is the only one of the four methods which is adequate. Many shielding applications fall in this class. In deep-penetration problems, anisotropic effects can dominate, thus requiring an accurate treatment of the anisotropy of both flux and cross section. It is well known that diffusion theory is not very accurate when used to calculate systems involving regions of very dissimilar cross-section values, such as is the case when control rods are interspersed in a reactor core. Because of the anisotropy involved in gamma-ray problems, S_n theory should be used.

Diffusion theory, on the other hand, is certainly the most successful of the four methods in terms of the amount of use it has for designing reactors, etc. In cases involving reasonably large, homogeneous regions, it is generally adequate, such as is the case for a large class of "reactor" applications. For most problems, the diffusion theory option should run appreciably faster than S_n theory, since it has essentially one equation to solve, versus number-of-angles equations for S_n theory. This equation also can be explicitly solved using a matrix inversion procedure, whereas the S_n theory requires a more time-consuming iterative procedure. However, in many cases with large numbers of groups (200 to 300), the greater fraction of the calculational time can be spent calculating the scattering source terms, which tends to lessen the impact of time spent on a more correct theory. (This same observation can also be made of the infinite medium and B_n method.)

The infinite medium option is the fastest of the four methods and can be used safely to perform calculations for large homogeneous regions, wherein the spectrum may be needed to collapse cross sections. This option only determines the first moment of the flux, and is, therefore, quite suspect for many applications, such as calculating diffusion coefficients.

The B_n option shares many of the same restrictions as the infinite-medium method; however, this treatment does (as its name implies) use a buckling approximation to account for leakage from the large homogeneous region, thereby giving higher order flux moments that can be used, for example, to determine diffusion coefficients.

F3.1.5 SELECTION OF OUTPUT CROSS-SECTION LIBRARY FORMATS

XSDRNPM will, on option, collapse cross sections and write the collapsed sets into four different formats:

1. ANISN[3] BCD Library,
2. ANISN[3] Binary Library,
3. CCCC[5] ISOTXS Library, or
4. AMPX[6] Working Library.

ANISN formats are used by ANISN (a 1-D discrete-ordinates code), by DOT[7] [a two-dimensional (2-D) discrete-ordinates code], and by MORSE[8] (a multigroup Monte Carlo code). The formats are quite comprehensive and can handle coupled neutron-gamma calculations, arbitrary orders of anisotropy, upscattering, etc. The major shortcoming of the format is its lack of internal documentation as to its structure (e.g., no provisions exist for specifying where a particular kind of cross section is located in the library or even if it is included). ANISN libraries can be produced in a free-form card-image BCD format or in a binary form.

The CCCC (Committee on Computer Code Coordination) ISOTXS file is a format for neutron cross sections that is one of several "standard interfaces" developed to facilitate the exchange of data between different computer codes. It is a self-defined format, which has provisions for identifying cross sections in the library. Scattering matrices can be supplied for elastic, inelastic, and (n,2n) scattering.

The choice of the output cross-section format is largely (if not totally) determined by the computer code that will use the data. However, in the interest of generality and maximum possible utilization of collapsed cross sections, note that XSDRNPM always produces an AMPX working library when cross sections are collapsed, and all other formats are produced by reformatting data from this library. In fact, stand-alone modules exist for converting AMPX working libraries to the ANISN formats and CCCC ISOTXS form and other formats. Therefore, for archival purposes, if a collapsed library is to be saved, the working format is the best choice, because it is the most general of those provided.

F3.2 THEORY AND PROCEDURES

This section describes the models and procedures which are employed in XSDRNPM.

F3.2.1 ONE-DIMENSIONAL DISCRETE-ORDINATES THEORY

The time-independent Boltzmann transport equation can be written:

$$\vec{\Omega} \cdot \nabla \psi(\vec{r},E,\vec{\Omega}) + \Sigma_t(\vec{r},E)\,\psi(E,\vec{r},\vec{\Omega}) = S(\vec{r},E,\vec{\Omega}) \ . \qquad \text{(F3.2.1)}$$

This expression is a balance condition that states simply that losses due to leakage (first term) and collisions (second term) must equal the source of neutrons, at some point in space $\vec{r}$, energy E, and in direction $\vec{\Omega}$ per unit volume and energy and solid angle. Other terms in the expression are $\Sigma_t(\vec{r},E)$, the total macroscopic cross section of the medium, which is typically assumed isotropic, and the flux, $\psi(\vec{r},E,\vec{\Omega})$.

The source term, $S(\vec{r},E,\vec{\Omega})$, has three components:

1. a scattering source, $S(\vec{r},E,\vec{\Omega})$
2. a fission source, $F(\vec{r},E,\vec{\Omega})$, and
3. a fixed source, $Q(\vec{r},E,\vec{\Omega})$.

The scattering source is given by:

$$S(\vec{r},E,\vec{\Omega}) = \int_0^{4\pi} d\vec{\Omega}' \int_0^{\infty} dE'\,\Sigma_s(\vec{r},E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega})\,\psi(\vec{r},E',\vec{\Omega}')) . \qquad \text{(F3.2.2)}$$

The fission source term, typically, is written

$$F(\vec{r},E,\vec{\Omega}) = \frac{1}{4\pi k}\chi(\vec{r},E) \int_0^{4\pi} d\vec{\Omega}' \int_0^{\infty} dE'\,\nu(\vec{r},E')\,\Sigma_f(\vec{r},E')\,\psi(\vec{r},E',\vec{\Omega}') , \qquad \text{(F3.2.3)}$$

where $\Sigma_s(\vec{r},E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega})$ is the macroscopic scattering cross section per unit energy for scattering from energy E' to E, $\chi(\vec{r},E)$ is the fraction of the fission neutrons per unit energy produced at $\vec{r}$ and E, $\nu(\vec{r},E)$ is the average number of neutrons produced per fission, $\Sigma_f(\vec{r},E)$ is the macroscopic fission cross section and k is the "effective multiplication constant." Note that, as in the case of the total cross-section value, χ, Σ_f, and υ have been assumed to be isotropic.

Three common coordinate systems are shown in Fig. 3.2.1. XSDRNPM is a 1-D code, which means that in the case of the slab, it is calculating at points along one axis where the system is assumed to extend to infinity along the other two axes. If we assume a calculation along the x-axis, this says that there is no leakage in the y or z directions, and our directions reduce to angles referenced to the x-axis. In the case of the cylinder, the length (z-axis) is infinite and the calculation is for points (shells) located at distance r from the central axis. For the sphere, the calculation is of shells located at radius, r, from the center of the spherical system.

Figure F3.2.2 illustrates the 1-D coordinate systems for slabs, cylinders, and spheres. Note that the directions are cones in the case of the slab and sphere, whereas in the case of the cylinder, the same simple

symmetries do not hold (a cone around the radius does not strike the next cylindrical shell at the same distance from a point on a radius) and the directions must be specifically described. Many symmetries in the 1-D cylinder, however, allow one to only describe directions for one quadrant of the direction sphere about a point as will be noted in Sect. F3.2.2.

The 1-D geometries allow considerable simplification to be made to Eq. (F3.2.1), especially in the leakage term $\vec{\Omega}\cdot\nabla\psi$. It is traditional to calculate as a function of angles expressed in cosine units; i.e., $\mu = \cos\phi$ and $\eta = \cos\xi$. This requires $\psi(x,E,\mu)$ for slabs, $\psi(x,E,\mu,\eta)$ for cylinders and $\psi(r,E,\mu)$ for spheres. Table F3.2.1 gives the form of the leakage terms for the three geometries.

Table F3.2.1 One-dimensional leakage terms

Geometry	$\vec{\Omega}\cdot\nabla\psi$
Slab	$\mu\frac{\partial\psi}{\partial x}$
Cylinder	$\frac{\mu}{r}\frac{\partial(r\psi)}{\partial r} - \frac{1}{r}\frac{\partial(\eta\psi)}{\partial\phi}$
Sphere	$\frac{\mu}{r^2}\frac{\partial(r^2\psi)}{\partial r} + \frac{1}{r}\frac{\partial[(1-\mu^2)\psi]}{\partial\mu}$

F3.2.2 MULTIGROUP ONE-DIMENSIONAL BOLTZMANN EQUATION

In multigroup schemes, the point-energy balance equations are converted to multigroup form by first selecting an energy structure and then writing a multigroup equivalent of the point equation which requires multigroup constants that tend to preserve the reaction rates that would arise from integrating the point equations by group. If we designate the groups by g, such that

$$\psi_g(x,\mu) = \int_g dE\,\psi(x,E,\mu) \qquad \text{(F3.2.4)}$$

and

$$\psi_g(x) = \int_{-1}^{1} d\mu\,\psi_g(x,\mu)\ , \qquad \text{(F3.2.5)}$$

then the following form of 1-D equation can be derived for the slab case:

$$\mu\frac{\partial\psi_g(x,\mu)}{\partial x} + \Sigma_t(x)\,\psi(x,\mu) = S_g(x,\mu) + F_g(x,\mu) + Q_g(x,\mu)\ . \qquad \text{(F3.2.6)}$$

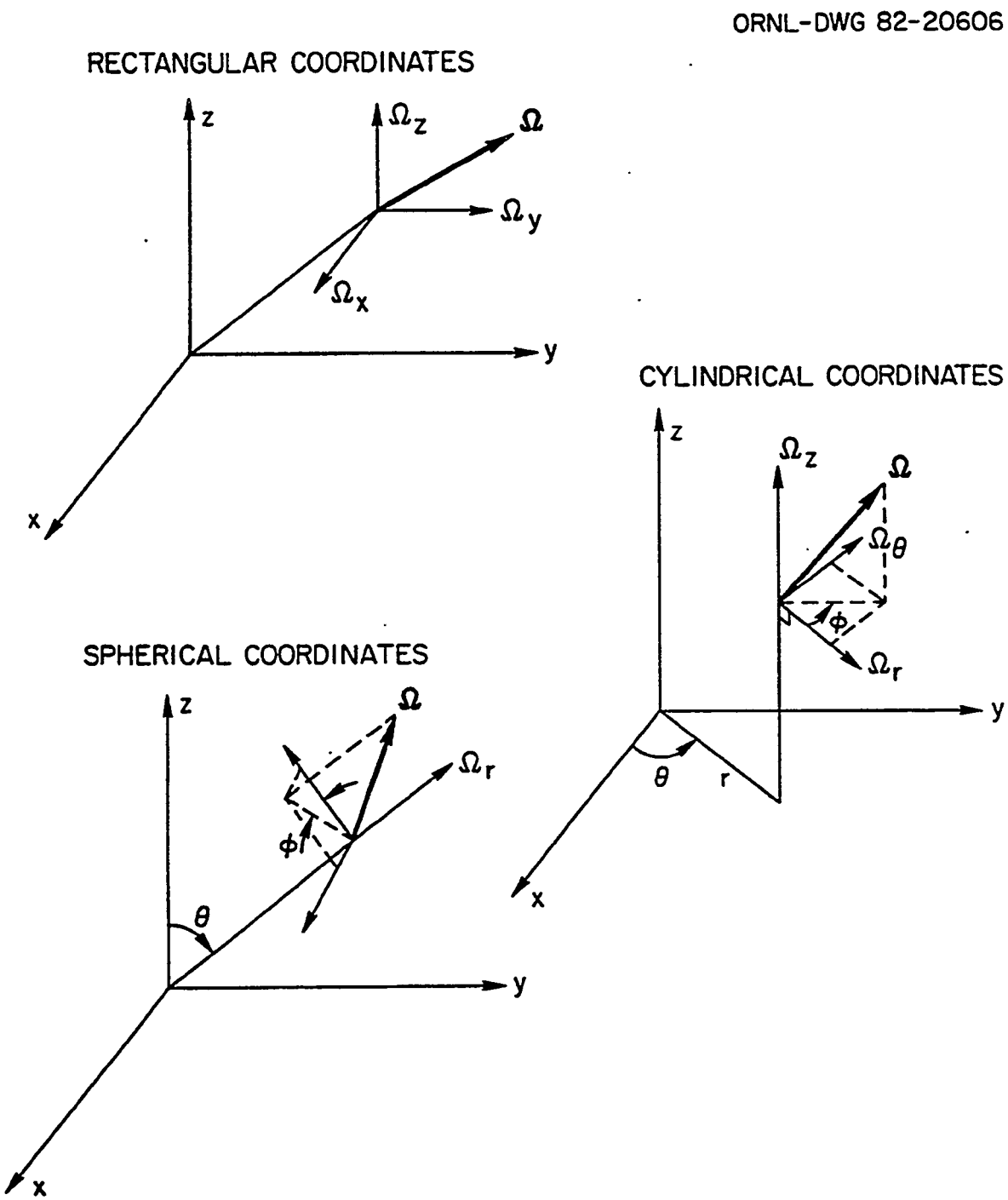


Figure F3.2.1 Three common coordinate systems

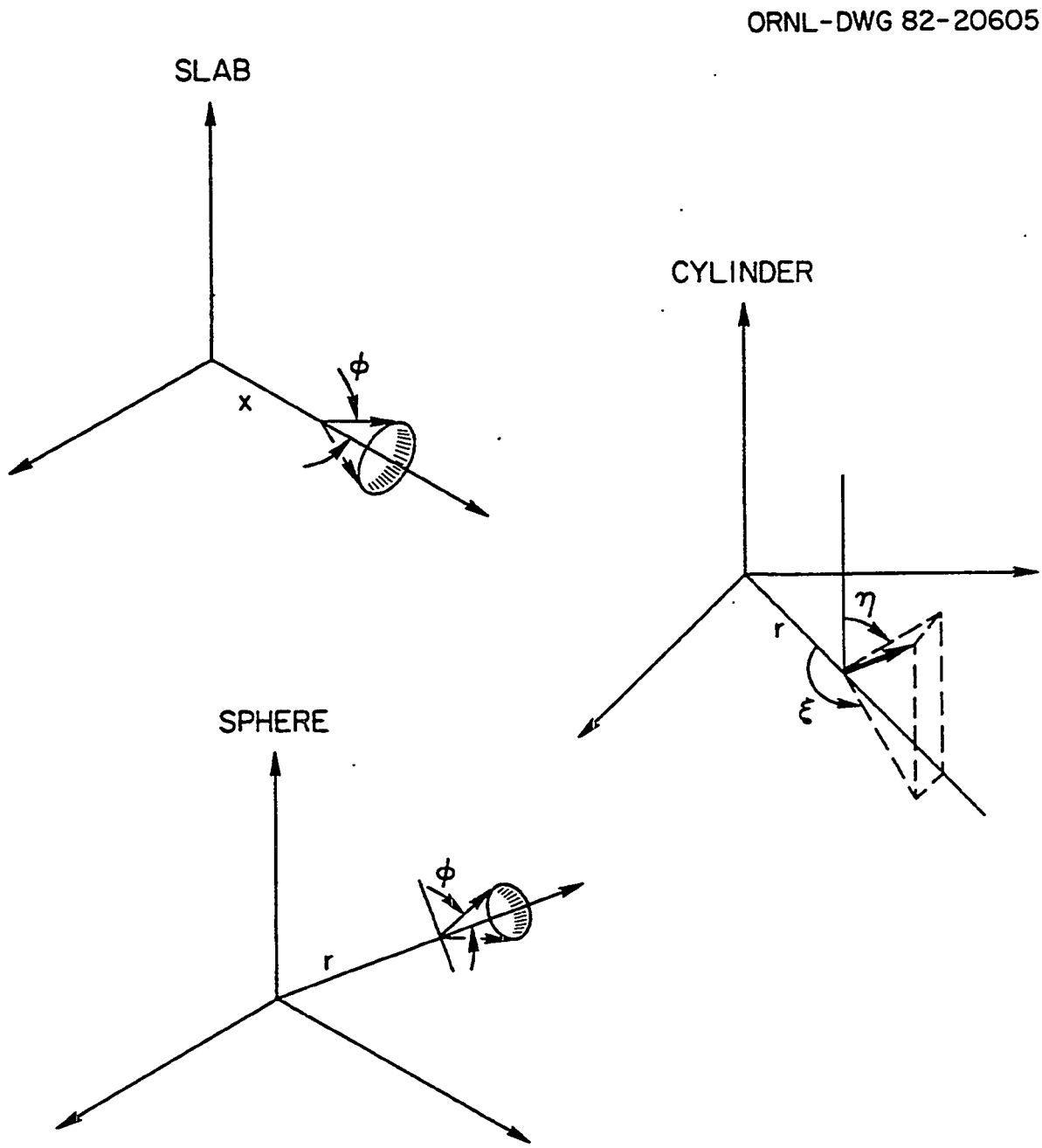


Figure F3.2.2 Three 1-D coordinate systems

The equations for the cylinder and sphere are essentially the same, in this notation, except for the differences in the leakage terms from Table F3.2.1.

In Eq. (F3.2.6), S_g, F_g, and Q_g are the scattering, fission, and fixed sources, respectively. The scattering term is discussed in Sect. F3.2.3. The multigroup form of the fission source is

$$F_g(x,\mu) = \frac{\chi_g}{2\pi k} \sum_{g'} \overline{\nu\Sigma_{fg'}}(x)\,\psi_{g'}(x), \qquad \text{(F3.2.7)}$$

where χ_g is the fraction of the fission neutrons that are produced in group g, and is the average of the product of υ, the average number of neutrons produced per fission and Σ_f, the fission cross section.

F3.2.3 SCATTERING SOURCE TERM

In discrete-ordinates theory, one typically calculates the Legendre moments of the flux, $\psi_{g,l}$, defined by

$$\psi_{g,l} = \frac{1}{2}\int_{-1}^{1} d\mu\,\psi_g(\mu)P_l(\mu)\ . \qquad \text{(F3.2.8)}$$

The group-to-group scattering coefficients are, themselves, fit with Legendre polynomials, such that

$$\sigma(g'\to g,\mu) = \sum_{l=0}^{ISCT} \frac{2l+1}{2}\,\sigma_l(g'\to g)P_l(\mu)\ . \qquad \text{(F3.2.9)}$$

In this example, we have a fit of order ISCT. [Note that ORNL cross-section libraries typically contain the $2l + 1$ factor in the $\sigma_l(g'\to g)$ matrix.]

F3.2.3.1. *Slab and Spherical Geometries*

Because of the symmetries in 1-D slabs and spheres, only one angle is needed to describe a "direction." In the case of the slab, the angle is taken with reference to the x-axis, while for the sphere, it is with reference to a radius vector between the point and the center of the sphere. This means that the flux can be expanded in ordinary Legendre polynomials, such that

$$\begin{aligned} \psi(r,E,\mu) &= \sum_{l=0}^{\infty} \psi_l(r,E)P_l(\mu) \\ \psi_l(r,E) &= \int_{-1}^{1} \frac{d\mu}{2}\,P_l(\mu)\psi(r,E,\mu). \end{aligned} \qquad \text{(F3.2.10)}$$

When Eq. (F3.2.10) and Eq. (F3.2.9) are introduced into Eq. (F3.2.2), the following expression is derived for the scattering source:

$$S(r,E,\mu) = 2\pi P_l(\mu)\int_0^{\infty} dE' \int_{-1}^{1} d\mu' \sum_{l=0}^{ISCT} \frac{2l+1}{2}\,\Sigma_{s_l}(r,E'\to E)P_l(\mu')\psi_l(r,E')\ , \qquad \text{(F3.2.11)}$$

where *ISCT* is the order of fit to the fluxes and cross sections.

F3.2.3.2 *Cylindrical Geometry*

The situation is more complicated in the case of the 1-D cylinder where the flux (and cross section) must be given as a function of two angles. Consider Fig. 3.2.3.

The addition theorem for associated Legendre polynomials can be used to transform from scattering angle coordinates to the real coordinates required in the cylindrical case:

$$P_l(\mu_0) = \sum_{n=-1}^{l} \frac{(l-n)!}{(l+n)!} P_l^n(\mu) P_l^n(\mu') e^{in(\zeta-\zeta')}, \qquad \text{(F3.2.12)}$$

where $\mu_0 = \cos\theta_{0,\mu} = \cos\theta$ and $\mu' = \cos\theta'$.

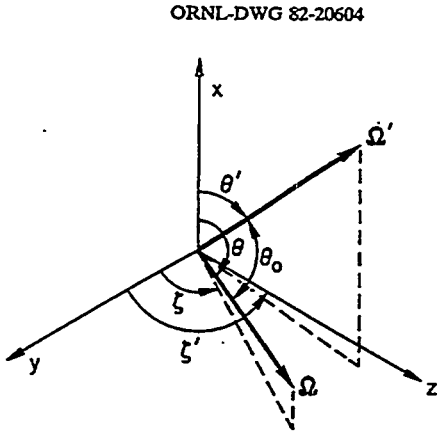


Figure F3.2.3 One-dimensional cylindrical scattering coordinates

If we note that

$$\sigma_s(r,E'\to E,\vec{\Omega}'\to\vec{\Omega}) = \sigma_s(r,E'\to E)P_l(\vec{\Omega}'\cdot\vec{\Omega})$$
$$= \sigma_s(r,E'\to E)P_l(\mu_0) \ ,$$

Eq. (F3.2.12) can be introduced into Eq. (F3.2.2) to yield

$$S(r,E,\mu) = \int_0^\infty dE' \int_{-1}^{1} d\mu' \int_0^{2\pi} d\zeta' \psi(\vec{r},E',\mu',\zeta') \sum_{l=0}^{ISCT} \frac{2l+1}{2} \sigma_{s_l}(\vec{r},E'\to E) \times \sum_{n=-l}^{l} \frac{(l-n)!}{(l+n)!} P_l^n(\mu) P_l^n(\mu') e^{in(\zeta-\zeta')} . \quad \text{(F3.2.13)}$$

Now it is convenient to recall that

$$\cos x = \frac{e^{ix}+e^{-ix}}{2}, \quad \text{(F3.2.14)}$$

which can be introduced into Eq. (F3.2.13) and rearranged to give

$$S(r,E,\mu) = \sum_{l=0}^{ISCT} \frac{2l+1}{2} \int_0^\infty dE' \, \sigma_{s_l}(\vec{r},E'\to E) \left[P_l(\mu) \int_{-1}^{1} d\mu' \int_0^{2\pi} d\zeta' \psi(\vec{r},E',\mu',\zeta') P_l(\mu') \right] + \sum_{n=1}^{l} 2 \frac{(l-n)!}{(l+n)!} P_l^n(\mu) \left[\int_{-1}^{1} d\mu' \int_0^{2\pi} d\zeta' \psi(\vec{r},E',\mu',\zeta') P_l^n(\mu') \cos[n(\zeta-\zeta')] \right] . \quad \text{(F3.2.15)}$$

We now define moments of the flux, ψ_l, by

$$\phi_l(\vec{r},E) = \int_{-1}^{1} d\mu' \int_0^{2\pi} d\zeta' \psi(\vec{r},E,\mu',\zeta') P_l(\mu') . \quad \text{(F3.2.16)}$$

It is also convenient to make use of the trigonometric relationship

$$\cos[n(\zeta-\zeta')] = \cos n\zeta \cos n\zeta' + \sin n\zeta \sin n\zeta' , \quad \text{(F3.2.17)}$$

which suggests two other sets of flux moments:

$$\psi_l^n(\vec{r},E) = \sqrt{2\frac{(l-n)!}{(l+n)!}} \int_{-1}^{1} d\mu' \int_0^{2\pi} d\zeta' \psi(\vec{r},E,\mu',\zeta') P_l^n(\mu') \cos n\zeta' \quad \text{(F3.2.18a)}$$

and

$$\psi_l^n(\vec{r},E) = \sqrt{2\frac{(l-n)!}{l+n)!}} \int_{-1}^{1} d\mu' \int_0^{2\pi} d\zeta' \psi(\vec{r},E,\mu',\zeta') P_l^n(\mu') \sin n\zeta' . \quad \text{(F3.2.18b)}$$

With a 1-D cylinder, the flux is symmetric in ζ; therefore, it is an even function, and the terms involving $\sin n\zeta$ will vanish. This fact yields the following expression for Eq. (F3.2.15):

$$S(r,E,\mu)=\sum_{l=0}^{ISCT}\frac{2l+1}{2}\int_0^\infty dE'\,\sigma_{s_l}(\vec{r},E'\to E)$$
$$\left[P_l(\mu)\psi_l(\vec{r},E')+\sum_{n=1}^{l}\sqrt{2\frac{(l-n)!}{(l+n)!}}P_n^l(\mu)\cos n\zeta\,\psi_l^n(\vec{r},E)\right]. \qquad \text{(F3.2.19)}$$

We observe further that for an even function in ζ, the odd l and odd (l-n) moments must all vanish, such that the following moments are nonzero for various orders of scattering:

ISCT	Nonzero Flux Moments
0	ψ_0
1	ψ_0,ψ_1^1
2	$\psi_0,\psi_1^1,\psi_2,\psi_2^2$
3	$\psi_0,\psi_1^1,\psi_2,\psi_2^2,\psi_3^1,\psi_3^3$
4	$\psi_0,\psi_1^1,\psi_2,\psi_2^2,\psi_3^1,\psi_3^3,$

In general, [ISCT(ISCT + 4)/4] + 1 moments are required.

F3.2.4 DISCRETE-ORDINATES DIFFERENCE EQUATIONS

In formulating the S_n equations, several symbols are defined which relate to a flux in an energy group g, in a spatial interval i, and in an angle m.

Typically, the flux is quoted as an integral of the flux in an energy group g, whose upper and lower bounds are E_g^U and E_g^L, respectively.

$$\psi_g = \int_{E_g^L}^{E_g^U} dE\,\psi(E)\ . \qquad \text{(F3.2.20)}$$

A mechanical quadrature is taken in space, typically IM intervals with IM + I boundaries. Likewise, an angular quadrature is picked compatible with the particular 1-D geometry, typically MM angles with associated directional coordinates and integration weights.

The different equations are formulated in a manner which involves calculating so-called angular fluxes, $\psi_{g,i,m}$, at each of the spatial interval boundaries, and also cell-centered fluxes, $\psi_{g,i+\frac{1}{2},m}$, at the centers of the

spatial intervals. The centered fluxes are related to the angular boundary fluxes by "weighted diamond difference" assumptions as will be described below.

Units on angular fluxes are per unit solid angle w_m and per unit area. Units on the centered fluxes are track length per unit volume of the interval. In both cases the fluxes are integrated in energy over the group g.

The areas and volumes for the three geometries are listed in Table F3.2.2.

Table F3.2.2 One-dimensional areas and volumes

Geometry	Area	Volume
Slab	1.0	$x_{i+1} - x_i$
Cylinder	$2\pi r_i$	$\pi(r_{i+1}^2 - r_i^2)$
Sphere	$4\pi r_i^2$	$4/3\ \pi(r_{i+1}^3 - r_i^3)$

F3.2.4.1 *Discrete-Ordinates Equation for a Slab*

Consider a spatial cell bounded by (x_i, x_{i+1}) and write the loss term for flow through the cell in direction μ_m. The net flow in the x-direction out the right side is the product of the angular flux times the area times the solid angle times the cosine of the angle:

$$w_m \mu_m A_{i+1} \psi_{g,i+1,m} .$$

The net loss from the cell is the dffference between the flow over both boundaries:

$$w_m \mu_m (A_{i+1} \psi_{g,i+1,m} - A_i \psi_{g,i,m}) . \qquad \text{(F3.2.21)}$$

The loss in the spatial cell due to collisions is given by the product of the centered angular flux (in per unit volume units) times the total macroscopic cross section times the solid angle times the volume:

$$w_m \sigma_{g,i+\frac{1}{2}} V_i \psi_{g,i+\frac{1}{2},m} . \qquad \text{(F3.2.22)}$$

The sources in direction μ_m are given by the product of the solid angle times the interval volume times the volume-averaged source (sum of fixed, fission, and scattering) in the direction m:

$$w_m V_i S_{g,i+\frac{1}{2},m} . \qquad \text{(F3.2.23)}$$

The slab equation is obtained by using Eqs. (F3.2.21), (F3.2.22), and (F3.2.23) and substituting proper values for area and volume:

$$w_m \mu_m (\psi_{g,i+1,m} - \psi_{g,i,m}) + w_m \sigma_{g,i+\frac{1}{2}} \psi_{g,i+\frac{1}{2},m} (x_{i+1} - x_i) = w_m S_{g,i+\frac{1}{2},m} (x_{i+1} - x_i) . \qquad \text{(F3.2.24)}$$

In an MM angle quadrature set, there are MM of these equations and they are coupled through the assumption on how the cell-centered flux relates to the boundary angular fluxes, the sources, and the boundary conditions, as will be discussed later.

F3.2.4.2 *Discrete-Ordinates Equations for Sphere and Cylinder*

The development of the equations for these geometries is analogous to that for the slab except that the leakage terms are more complicated. Consider Fig. F3.2.4.

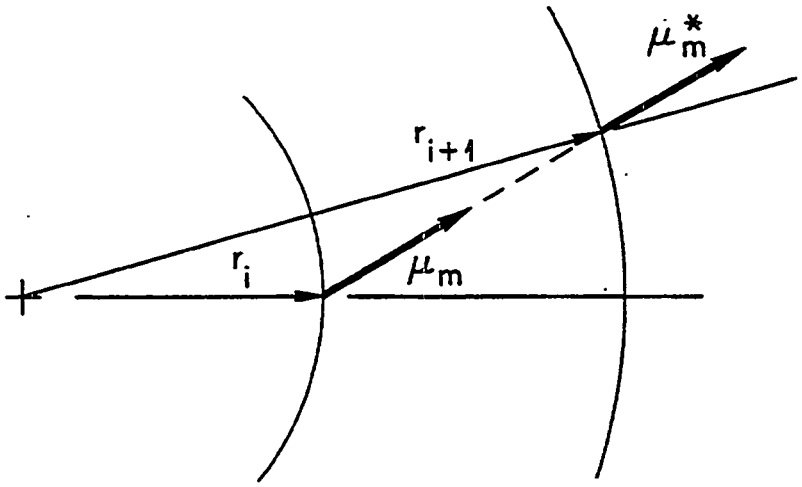


Figure F3.2.4 Angular redistribution in spherical geometry

Recall that the directions are taken with reference to the radius vector for a sphere. A particle traveling in direction μ_m at r_i will intersect the radius vector to the next point r_{i+1} at a different angle μ_m^*. The same effect also exists for the cylinder, though in this case the direction coordinates are more complicated. Because of the effect, a loss term is included for the "angular redistribution." It is defined in a manner analogous to Eq. (F3.2.21) as

$$\alpha_{i+\frac{1}{2},m+\frac{1}{2}} \psi_{g,i+\frac{1}{2},m+\frac{1}{2}} - \alpha_{i+\frac{1}{2},m-\frac{1}{2}} \psi_{g,i+\frac{1}{2},m-\frac{1}{2}}, \qquad \text{(F3.2.25)}$$

where the α coefficients are to be defined in such a manner as to preserve particle balance. In this case one speaks of $m + \frac{1}{2}$ and $m - \frac{1}{2}$ as the corresponding angles to μ_m on the i + 1*th* and i*th* boundaries, respectively. (See Fig. F3.2.5.) Here we are interested in an angle μ_m at the center of interval i which redistributes to $\mu_{m-\frac{1}{2}}$ at boundary i and to $\mu_{m+\frac{1}{2}}$ at boundary i + 1.

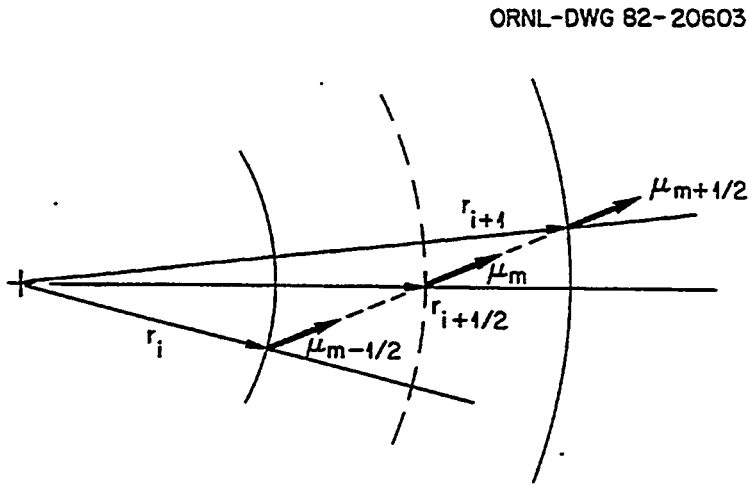


Figure F3.2.5 Angular redistribution

Obviously, it is necessary that the net effect of all redistributing be zero, in order to maintain particle balance. This condition is met if

$$\sum_{m=1}^{MM} \alpha_{m-\frac{1}{2}} \psi_{m-\frac{1}{2}} + \alpha_{m+\frac{1}{2}} \psi_{m+\frac{1}{2}} = \alpha_{\frac{1}{2}} \psi_{\frac{1}{2}} + \alpha_{MM+\frac{1}{2}} \psi_{MM+\frac{1}{2}} = 0 , \qquad \text{(F3.2.26)}$$

where we have dropped the group and interval indexes.

In order to develop an expression for determining the α's, consider an infinite medium with a constant isotropic flux. In this case, there is no leakage and the transport equation reduces to

$$\Sigma_t \phi = S . \qquad \text{(F3.2.27)}$$

This condition requires that

$$\mu_m w_m (A_{i+1} \psi_{g,i+1,m} - A_i \psi_{g,i,m}) + \alpha_{i+\frac{1}{2},m+\frac{1}{2}} \psi_{g,i+\frac{1}{2},m+\frac{1}{2}} - \alpha_{i+\frac{1}{2},m-\frac{1}{2}} \psi_{g,i+\frac{1}{2},m-\frac{1}{2}} = 0 , \qquad \text{(F3.2.28)}$$

which when we note that all the ψ terms in the infinite medium case are equal becomes

$$\mu_m w_m (A_{i+1} - A_i) = -\alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}} , \qquad \text{(F3.2.29)}$$

which is a recursion relationship for α.

From Eq. (F3.2.26) we see that the conservation requirement can be met if

$$\alpha_{\frac{1}{2}} = \alpha_{MM+\frac{1}{2}} = 0 \qquad \text{(F3.2.30)}$$

for any values of flux, and is, therefore, used to evaluate the α's along with Eq. (F3.2.28) or (F3.2.29). (Note that had we included the redistribution term in the slab equation, Eq. (F3.2.29) would have given zeroes for the terms, which is as one would expect for this geometry.)

The final discrete-ordinates expression for spheres and cylinders is then derived by summing expressions (F3.2.21), (F3.2.25), (F3.2.22) and setting it equal to expression (F3.2.23).

F3.2.4.3 *S_n Quadratures for Slabs*

XSDRNPM will automatically calculate quadrature sets for each of the 1-D geometries, or a user can, if he wants, input a quadrature.

In the case of the 1-D slab, the quadrature is a double Gauss-Legendre set based on recommendations from Ref. 9.

The ordering of the directions for a slab is shown in Fig. F3.2.6.

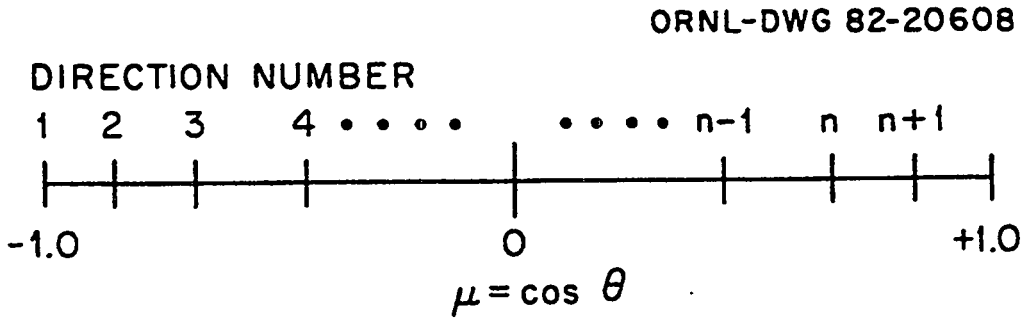


Figure F3.2.6 Ordering of S_n directions for slabs and spheres

Note that in referring to the quadratures for any of the geometries, we do not attempt to define an explicit area on a unit sphere, but rather speak of characteristic directions with associated weights. In the case of the slab, it is convenient to think of "directions" which are shaped like cones, because of the azimuthal symmetry around the x-axis.

In an *nth* order quadrature, there are n + 1 angles with the first angle being taken at $\mu = -1.0$. This first angle is not required for the slab, but is needed for the curvilinear geometries because of the angular redistribution terms, as will be noted later. It is included in the slab case for reasons of uniformity of programming, etc.

Several requirements are made regarding the angles and weights in the quadrature set.

The arguments relating to angular redistribution can be expected to show that

$$\sum_{m=1}^{MM} \mu_m w_m = 0.0 \ . \qquad \text{(F3.2.31)}$$

This situation is ensured if the weight of the $\mu = -1.0$ direction is zero and the other directions and weights are symmetric about $\mu = 0$. (The $\mu = 0$ direction is never included in the quadrature set because of its singularity.)

Further, it is required that

$$\sum_{m=1}^{MM} w_m = 1.0 . \qquad \text{(F3.2.32)}$$

F3.2.4.4 *S_n Quadratures for Spheres*

The quadratures generated for spheres are Gauss-Legendre coefficients as recommended by Ref. 9. The ordering and symmetry requirements for spheres are the same as for slabs.

In the case of the sphere, the initial ($\mu = -1.0$) direction is required, because the difference equations involve three unknown values for each direction, μ_m: ψ_m and the fluxes at the two "redistributed" angles $\psi_{m-½}$ and $\psi_{m+½}$. It is obvious that an angle along the radius will not involve the redistribution; hence, the expression for this direction involves only $\psi(\mu = -1.0)$ as unknowns. Angle 2 proceeds by assuming $\psi_{2-½}$ is given by $\psi_1$and also uses a weighted diamond difference model to relate $\psi_m, \psi_{m-½}$ and $\psi_{m+½}$, as will be described below. Subsequent angles will then have values for $\psi_{m-½}$ calculated by the previous angle equations.

F3.2.4.5 *S_n Quadratures for Cylinders*

The quadrature sets for cylinders are more complicated (see Fig. F3.2.2) because the directions must be specified with two angles, ζ and η, where $\mu \equiv \sin \eta \cos \zeta$ and $\beta \equiv \cos \eta$.

In this case, practice is to use n/2 levels of directions for an n*th* order set. The levels correspond to fixed values of η. The number of angles by level starts with three in level 1, five in level 2, seven in level 3, etc. (Note that since cylindrical geometry is curvilinear, each level will start with a $\zeta = \pi$ direction that has zero weight for reasons analogous to those given for the spherical case. Figure F3.2.7 shows the ordering of the directions for an S_6 quadrature set. Angles 1, 4, and 9 are the starting directions (zero weight) for the levels.

In general, an n*th* order quadrature will contain n(n + 4)/4 angles. The cosines, μ, and the weights are stored in two arrays internally in the code; and, since the weights for the 1*st*, 4*th*, and 9*th* angles are zero, the cosines for the corresponding levels are placed in these locations in the arrays.

The cylindrical sets are based on Gauss-Tschebyscheff schemes as recommended by Ref. 9 with Gaussian quadratures in β and Tschebyscheff quadratures in μ.

F3.2.5 WEIGHTED-DIFFERENCE FORMULATION FOR DISCRETE-ORDINATES EQUATIONS

In order to solve the discrete-ordinates equations, an assumption is required concerning the relationship of the various flux terms: $\psi_{i,m}$, $\psi_{i+1,m}$, $\psi_{i+½,m}$, $\psi_{i,m-½}$, $\psi_{i+1,m-½}$.

The solution of the equations involves three major loops: an outer loop over energy groups, a loop over angles, and a loop over the spatial mesh. The spatial loop is made either from the origin to the outside boundary or from the outside to the origin, depending on whether the angle is directed outward or inward, respectively.

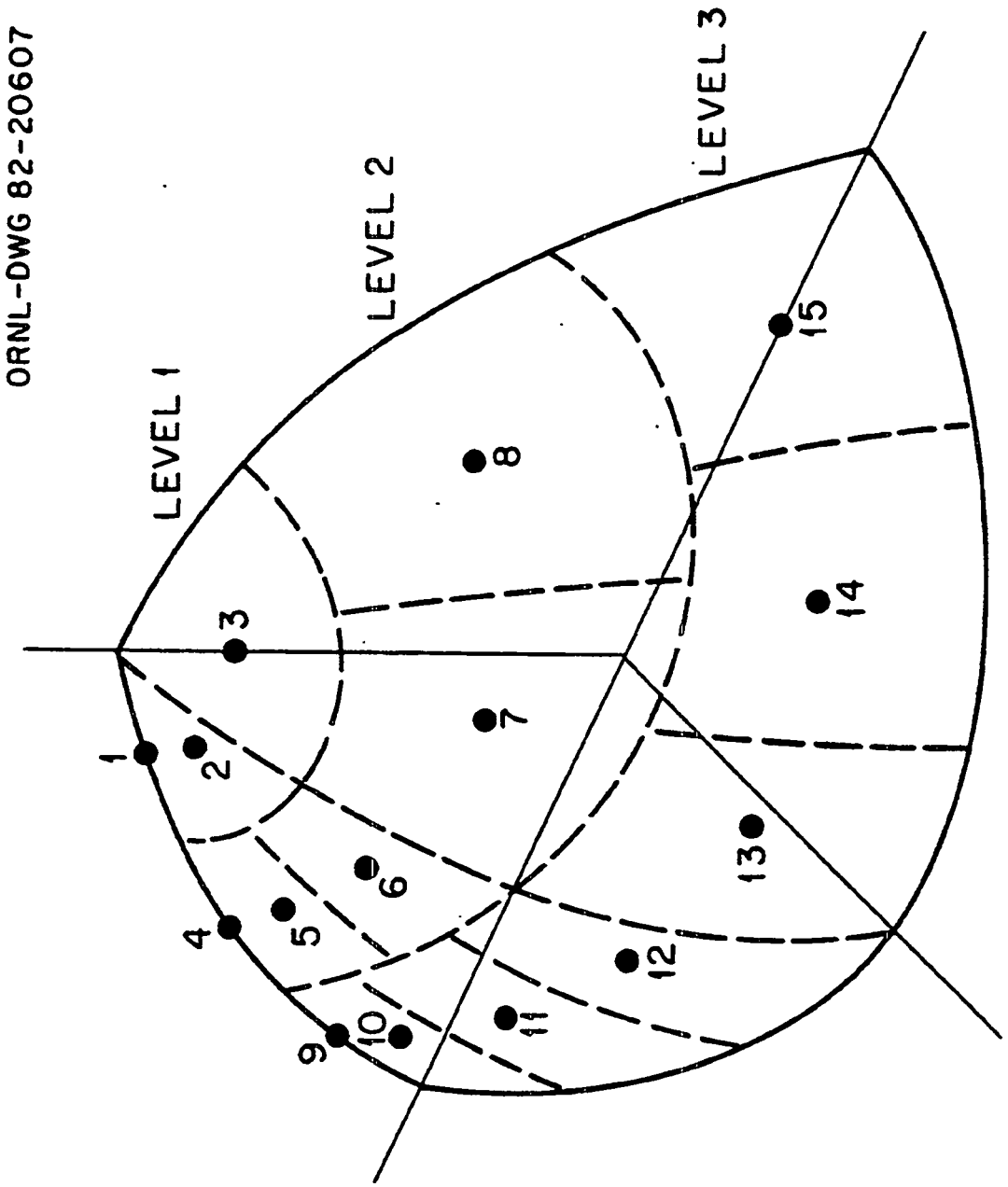


Figure F3.2.7 Ordering of the directions for an S_6 cylindrical set

Two models are widely used for expressing flux relationships: (1) the step model and (2) the diamond-difference linear model.

The "step model" is a histogram model whereby one sets the centered flux value to the appropriate boundary value, depending on which way the mesh sweep is going. If, for example, the sweep is to the right in space, then

$$\psi_{i+\frac{1}{2},m} = \psi_{i,m} ,$$

or if to the left,

$$\psi_{i+\frac{1}{2},m} = \psi_{i+1,m} .$$

Likewise, in angle:

$$\psi_{i+\frac{1}{2},m} = \psi_{i+\frac{1}{2},m-\frac{1}{2}} .$$

The step model involves a very crude approximation, but has the marked advantage of helping to ensure positivity of flux values as long as scattering sources are positive.

In the "diamond-difference" model, the centered fluxes are assumed linear with the edge values:

$$\psi_{i+\frac{1}{2}} = 0.5\ (\psi_i + \psi_{i+1})$$

$$\psi_m = 0.5\ (\psi_{m-\frac{1}{2}} + \psi_{m+\frac{1}{2}}) .$$

Unfortunately, though the linear model is clearly a better model than the step model, care must be taken by selecting a fine spatial mesh, or the linear extrapolation can lead to negative flux values. In some cases, the situation is so severe that it is impractical to take enough mesh points to eliminate the problems. Because of these difficulties XSDRNPM uses a different approach, as described below.

The weighted diamond difference model[10] was developed in an attempt to take advantage of the "correctness" of the linear model, while retaining the positive flux advantages of the step model.

A solution in some S_n codes is to use the linear model in all cases where positive fluxes are obtained and to revert to step model otherwise. Unfortunately, this method leads to artificial distortions in the fluxes.

Note that if one writes

$$\psi_{i+\frac{1}{2}} = a\psi_i + (1-a)\psi_{i+1} \qquad \text{(F3.2.33)}$$

$$\psi_m = b\psi_{m-\frac{1}{2}} + (1-b)\psi_{m+\frac{1}{2}} \qquad \text{(F3.2.34)}$$

that the same expression can be used to express linear or step model (e.g., $a = b = \frac{1}{2}$ is equivalent to linear, while a = b = 1.0 can be used for the step model).

In the weighted model, the intention is to use the linear model when fluxes are positive but to select values for a and b in the range

$$\frac{1}{2} \le a \text{ or } b \le 1.0 \qquad \text{(F3.2.35)}$$

that ensure positivity, if the source is positive.

At this point, it is convenient to rewrite the discrete-ordinates expression in a simplified notation, without the obvious subscripts on energy group, angle, etc.

$$w\mu(A_{i+1}\psi_{i+1} - A_i\psi_i) + \alpha_{m+½}\psi_{m+½} - \alpha_{m-½}\psi_{m-½} + w\sigma V\psi = wVS. \quad \text{(F3.2.36)}$$

Combining Eqs. (F3.2.36) and (F3.2.33) or (F3.2.34) yields the following expressions for ψ_{i+1} and $\psi_{m+½}$:

$$\psi_{i+1} = \frac{SV + C_2\psi_{m-½} + [\mu A_i - (1-a)D_1]\psi_i}{aD} \quad \text{(F3.2.37)}$$

$$\psi_{m+½} = \frac{SV + C_1\psi_i + \left[\frac{\alpha_{m-½}}{w} - (1-b)D_2\right]\psi_{m-½}}{bD}, \quad \text{(F3.2.38)}$$

where

$$C_1 = \mu\left[A_i + A_{i+1}\left(\frac{1}{\alpha} - 1\right)\right] \quad \text{(F3.2.39)}$$

$$C_2 = \frac{\alpha_{m-½}}{w} + \frac{\alpha_{m+½}}{w}\left(\frac{1}{b} - 1\right) \quad \text{(F3.2.40)}$$

$$D = \Sigma V_i + \frac{\mu A_{i+1}}{a} + \frac{\alpha_{m+½}}{wb} \quad \text{(F3.2.41)}$$

$$D_1 = D - \frac{\mu A_{i+1}}{a} \quad \text{(F3.2.42)}$$

$$D_2 = D - \frac{\alpha_{m+½}}{wb}. \quad \text{(F3.2.43)}$$

In determining a and b, the "theta-weighted" model uses arbitrary multipliers θ_s on SV and θ_n on the $C_2\psi_{m-½}$ or $C_1\psi_i$ terms in Eqs. (F3.2.37) and (F3.2.38). (In Ref. 11, a thorough discussion is given on the history of using different choices of θ_s and θ_n and the advantages and disadvantages of each method.) In XSDRNPM, a value of 0.9 is used for θ_s and θ_n following the practice in the DOT-IV code.[7]

$$[\mu A_i - (1-a)D_1]\psi_i < SV + C_2\psi_{m-½}, \quad \text{(F3.2.44)}$$

For ψ_{i+1} in (F3.2.37) to be positive, the numerator should be positive, thereby requiring which in the θ-weighted case becomes

$$[\mu A_i - (1-a)D_1]\psi_i < SV\theta_s + C_2\psi_{m-\frac{1}{2}}\theta_n \ . \qquad \text{(F3.2.45)}$$

A similar expression can be written for b using Eq. (F3.2.38).

For reasons of accuracy, it is desirable to use $a = b = \frac{1}{2}$. Therefore, when a or b is determined to be less than ½, it is automatically set to ½.

F3.2.6 BOUNDARY CONDITIONS

XSDRNPM allows a boundary condition to be specified for each of the two "outside" boundaries of its 1-D geometries. The options are the following:

1. Vacuum boundary - all angular fluxes that are directed inward at the boundary are set to zero (e.g., at the left-hand boundary of slab, $\psi(\mu>0) = 0$, etc.).

2. Reflected boundary - the incoming angular flux at a boundary is set equal to the outgoing angular flux in the reflected direction (e.g., at the left-hand boundary of a slab),

$$\psi_{in}(\mu) = \psi_{out}(-\mu) \ .$$

3. Periodic boundary - the incoming angular flux at a boundary is set equal to the outgoing angular flux in the same angle at the opposite boundary.

4. White boundary - the angular fluxes of all incoming angles on a boundary are set equal to a constant value such that the net flow across the boundary is zero, that is,

$$\psi_{in} = \frac{\sum_{m}^{out} w_m \mu_m \psi_m}{\sum_{m}^{in} w_m |\mu_m|} \ .$$

This boundary condition is generally used as an outer-boundary condition for cell calculation of cylinders and spheres that occur in lattice geometries.

5. Albedo boundary - this option is for the white boundary condition except that a user-supplied group-dependent albedo multiplies the incoming angular fluxes. This option is rarely used, as it is difficult to relate to most practical situations.

F3.2.7 FIXED SOURCES

Two types of inhomogeneous or fixed sources can be specified in XSDRNPM.

In the first case, an isotropic group-dependent volumetric source can be specified for any or all spatial intervals in a system.

In the second case, an angle- and group-dependent boundary source can be specified for any or all boundaries between spatial intervals in a system, excepting the left-most boundary. In this case, one specifies not a source but a flux condition on the boundary. If one uses the "track length" definition for flux, it is easy to show that the flux condition is related to a source condition by

$$\psi_m^\delta = \frac{S_m}{\mu_m} \ . \qquad \text{(F3.2.46)}$$

(This equation says that an isotropic source on a boundary would be input as a constant divided by the cosine of the direction.)

In fixed-source calculations, the total fixed source in the system can be normalized to an input parameter, XNF. In the volumetric source case, the source values will be normalized such that

$$XNF = \sum_{g=1}^{IGM} \sum_{i=1}^{IM} Q_{g,i} V_i , \qquad \text{(F3.2.47)}$$

and in the boundary source case,

$$XNF = \sum_{g=1}^{IGM} \sum_{i=1}^{IM} A_{i+1} \sum_{m=1}^{MM} \mu_m \psi_m^\delta(g,i) w_m \ . \qquad \text{(F3.2.48)}$$

In the case where both volumetric and boundary sources are specified, the two sums are normalized to XNF.

F3.2.8 DIMENSION SEARCH CALCULATIONS

XSDRNPM has three options for searching for dimensions such that the system will produce a specified effective multiplication factor, k_{eff}. The options are selected by a parameter IEVT in the 1$ array and are as follows:

1. zone width search (IEVT = 4),
2. outer radius search (IEVT = 5),
3. buckling search (IEVT = 6).

By default, the search is made to produce a k_{eff} value of unity. For k_{eff}'s other than unity, IPVT (3$ array) is set to unity and the desired k_{eff} is input as PV (5* array).

Other input parameters which apply specifically to all search calculations are in the 5* array and are EV, the starting eigenvalue guess, EVM, the eigenvalue modifier, EQL, the eigenvalue convergence, and XNPM, the new parameter modifier. These parameters are discussed in more detail below.

F3.2.8.1 *Zone-Width Search (IEVT = 4)*

With this option, one can vary the width of any or all zones in a case. Note that it is also possible to change zone widths at different rates.

This option requires the inputting of a zone width modifier array (41*) which is used to specify the relative movements of the zones according to the following expression:

$$\Delta Z_j^f = \Delta Z_j^i (1 + EV^* ZM_j),$$

where ΔZ_j^i, ΔZ_j^f are the initial and final widths of zone j, respectively, ZM_j is the zone width modifier for the zone (as input in the 41* array), and EV is the final "eigenvalue" for the problem. Note that a zero value for ZM wig specify a fixed zone width. Negative values for ZM are allowed.

F3.2.8.2 *Outer Radius Search (IEVT = 5)*

With this option, all zones are scaled uniformly in order to make the system attain the specified k_{eff}. The final zone widths are found by multiplying the initial values by the final "eigenvalue:"

$$\Delta Z_j^f = EV(\Delta Z_j^i) .$$

F3.2.8.3 *Buckling Search (IEVT=6)*

This option is used to search for "transverse" dimensions that will yield a specified k_{eff} for a system. This means that the search is for the height for a 1-D cylinder or the y- and/or z-dimensions in a 1-D slab.

For this option, the final dimensions are given by

$$\mathrm{DY} = DY_0 \times \mathrm{EV},$$

and

$$\mathrm{DZ} = DZ_0 \times \mathrm{EV},$$

where DY_0, DZ_0 are the initial dimensions input in the 5* array.

F3.2.8.4 *Search Calculation Strategy*

All the "dimension searches" use the same simple strategy. The calculations start by using the input eigenvalue (EV from the 5* array) to determine initial dimensions for the system. These dimensions allow the code to calculate a k_{eff}. The eigenvalue modifier (EVM in the 5* array) is then used to change the dimensions as follows:

IOPT = 4 (Zone width search)

$$\Delta Z_j^f = \Delta Z_j^i [1 + (EVM + EV)^* ZM_j]$$

IOPT = 5 (Outer radius search)

$$\Delta Z_j^f = \Delta Z_j^i [1 - 0.1^* (EVM + EV)]$$

IOPT = 6 (Buckling search)

$$\mathrm{DY} = DY_0 (\mathrm{EV} + \mathrm{EVM})$$
$$\mathrm{DZ} = DZ_0 (\mathrm{EV} + \mathrm{EVM}) .$$

The new dimensions are then used in a new calculation which determines a second k_{eff} value.

XSDRNPM searches for a unity value of k_{eff} by default; however, when IPVT = 1 (3$ array), a nonunity value can be specified in PV (5* array) and the search will be made on this value.

Once the two k_{eff}'s are known, which are based on eigenvalues of EV and EV + EVM, respectively, a linear fit is used to project to the next value for EV. This yields an expression of the form

$$EV_{next} = EVM\frac{(PV - k_1)}{(k_2 - k_1)} + EV,$$

where k_1 and k_2 are the first and second value of k_{eff}, respectively. After this iteration, the procedure is to fit a quadratic to the three most recent k_{eff} values in order to obtain an estimate for the next EV.

The procedure continues until a relative convergence of EQL (5* array) or better is obtained on EV.

To prevent oscillations in the search, extrapolations are limited by XNPM, the new parameter modifier from the 5* array.

F3.2.9 ALPHA SEARCH

It is possible to make some of the searches described in F3.2.8 in a more "direct" fashion than the strategy described in F3.2.8.4. XSDRNPM has two such options: (1) the alpha search and (2) a direct buckling search. These are described below.

F3.2.9.1 *Alpha Search*

The time-dependent form of the Boltzmann equation is identical with Eq. (F3.2.1), except for the inclusion of a time-gradient term on the left-hand side:

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t}.$$

All other flux terms in the expression also would include the time (t) argument.

In some analyses it is reasonable to assume that the time variation of the flux is exponential, that is,

$$\psi(\vec{r},E,\vec{\Omega},t) = \psi(\vec{r},E,\vec{\Omega})e^{\alpha t}.$$

When this variation is introduced into the expanded form of Eq. (F3.2.1), the exponential terms all cancel leaving a leading term:

$$\frac{\alpha}{v}\psi(\vec{r},E,\vec{\Omega}),$$

which is in the same form as the $\Sigma_t\psi$ term.

If one considers integrating over energy, angle, and space, the following expression can be derived:

$$P - A - L - \alpha V = 0,$$

where

P ≡ production in the system,
A ≡ absorptions in the system,
L ≡ leakage from the system,

$$V \equiv \int_0^\infty dE \int_0^{4\pi} d\vec{\Omega} \int_{system} d\vec{r}\, \frac{\psi(\vec{r},E,\vec{\Omega})}{v} .$$

Since all terms other than α can be determined from a calculation, it is possible to determine α directly, thereby avoiding a scheme like that used for dimension searches. In the balance expression, the fission component of the production term is adjusted for the case of a nonunity k_{eff} value (IPVT = 1 in the 3$ array).

An α-search has several practical applications. If, for example, a subcritical assembly is pulsed by a source, the time-dependence of the flux is expected to die off exponentially. Another way to interpret the α-value is as that amount of $1/v$ absorber which could be added or taken away from a system in order to achieve criticality. This number could be of interest when certain control materials are used, such as $^{10}B_5$, which is a "$1/v$" material.

F3.2.9.2 *Direct-Buckling Search*

A "direct-"buckling search can be made using a procedure analogous to that described in Sect. (F3.2.9.1). Recall that the buckling is introduced in order to represent a transverse leakage through the use of a $DB^2\psi$ term. This suggests that the foregoing balance expression be written:

$$P - A - L - \alpha DB^2 X = 0 ,$$

where

$$X \equiv \int_0^\infty dE \int_0^{4\pi} d\vec{\Omega} \int_{system} d\vec{r}\, \psi(\vec{r},E,\vec{\Omega}) .$$

In this case, the diffusion coefficients, D_g, are determined from

$$D_g = \frac{1}{3\Sigma_{tr_g}} ,$$

where

$$\Sigma_{tr_g} = \Sigma_{t_g} - \Sigma_{1_g} ,$$

and Σ_1 is determined from the P_1 scattering matrices:

$$\Sigma_{1_g} = \sum_{g'} \Sigma_1(g \to g') .$$

The original B^2 value is determined as specified in Sect. F3.2.12, and the α is a search parameter that one multiplies by the original B^2 value in order to determine the final buckling and, hence, the dimensions of the system.

F3.2.10 ITERATION AND CONVERGENCE TESTS

Two parameters are used to specify the required levels of convergence on an XSDRNPM calculation. These are EPS and PTC, both given in the 5* array. The flux calculations proceed through a series of iterations until either convergence is achieved or the specified iteration limit is exceeded.

The basic iteration strategy in XSDRNPM is now described. The discrete-ordinates difference equation is solved for the first angle and the first energy group. This sweep generally is made from the last interval boundary to the center of the system, and it uses the flux guess supplied as part of the input along with the boundary conditions. The second angle is then calculated, etc., until all angles in the quadrature are treated. At the end of this sweep, new scalar fluxes for the midpoints of all intervals have been determined. The angular sweep continues until either the point scalar fluxes are converged to within PTC or until the code makes IIM inner iterations. An exception to this "inner iteration" pattern occurs on the first outer (defined below) iteration whenever a fission density guess is used, instead of the flux guess. In this case, the program uses 1-D diffusion theory to determine a scalar flux value for all intervals and the angular sweeps are not made until the second outer iteration. After the first group is completed, the calculation goes to the second group and repeats the above procedure. This continues until all groups have been treated.

The pass through all groups, angles, and intervals is called an outer iteration. Most of the convergence checks on the outer iteration have to do with reaction rates involving all energy groups and are made against the EPS parameter mentioned above. For a coupled neutron-gamma problem, outer iterations are only performed for the neutron groups until convergence is achieved, then the final converged pass is made over all groups. In discussing these checks, it is convenient to define several terms:

$Q \equiv$ total fixed source in the system

$F \equiv$ total fission source in the system

$D \equiv$ total outscatter rate in the system

$$D \equiv \sum_{i}^{intervals} \sum_{g}^{groups} \sum_{g' \neq g}^{groups} \psi_{i,g} \sigma_{g-g'} v_i$$

$\psi_{i,g} \equiv$ scalar flux in intervals i and group g

$\sigma_{g-g'} \equiv$ macroscopic scattering cross section from group g to group g′

$v_i \equiv$ volume of interval i

$k \equiv$ outer iteration number

$IGM \equiv$ total number of energy groups

$Q_g \equiv$ fixed source in group g

$F_g \equiv$ fission source in group g

$$\epsilon_g' \equiv \frac{Q_g + F_g}{IGM} * \text{EPS}$$

$$\lambda_k \equiv \frac{Q + F_k}{Q + F_{k-1}}$$

$$G_k \equiv \frac{D_k}{Q+F_k}$$

$$\lambda_k' \equiv \frac{G_{k-1}}{G_k}$$

$U_k \equiv$ total upscatter rate $= \sum_i \sum_g \sum_{g'<g} \psi_{i,g}\sigma_{g'\to g}\nu_i$

An inner iteration in XSDRNPM consists of sweeping one time through the entire spatial mesh for all the S_n angles for one energy group.

When the fluxes for a particular group are being calculated, inner iterations will continue until (a) the number of inner iterations for this outer iteration exceeds IIM, the inner iteration maximum, or (b) until the following criteria are met.

$$(1) \quad \sum_{\substack{i \\ intervals}} |(\psi_{i,g}^k - \psi_{i,g}^{k-1})|\, \sigma_{g'\to g}\nu_i \le \epsilon_g' .$$

$$(2) \quad \sum_i |(\psi_{i,g}^k - \psi_{i,k}^{k-1})|\, (\sigma_t - \sigma_{g\to g})V_i \le \epsilon_g' .$$

And, if PTC, the point flux convergence criterion, is input greater than zero, XSDRNPM also requires

$$(3) \quad \max_i \left| \frac{\psi_{i,g}^k - \psi_{i,g}^{k-1}}{\psi_{i,g}^k} \right| \le PTC .$$

At the end of an outer iteration, the following checks are made:

$$(4) \quad |1.0 - \lambda_k| \le EPS .$$

$$(5) \quad R|1.0 - \lambda_k'| \le EPS .$$

R is a convergence relaxation factor and is set internally to 0.5 in XSDRNPM. If all convergence criteria are met, if ICM, the outer iteration maximum, is reached, or if ITMX, the maximum execution time, is exceeded, the problem will be terminated with full output; otherwise, another outer iteration will be started.

F3.2.11 GROUPS BANDING (SCALING REBALANCE)

As described above, the normal mode of operation in XSDRNPM is to do inner iterations on a group until it converges, then go to the next group. For groups where there is no upscatter, the scattering source to a group depends only on higher energy groups for which the fluxes have already been calculated. A fixed source problem with no fission and no upscattering can, therefore, be converged in one outer iteration. Since fission sources and upscattering sources are calculated with fluxes from the previous outer iteration, multiple outer iterations must be done to converge problems involving these kinds of sources. For problems involving many fine thermal groups (groups with both upscatter and downscatter), a special convergence problem arises. Because the groups are fine, within-group scattering is small and the flux calculation is dominated by scattering

sources from other groups. This situation leads to a very slow reduction in scattering source errors from one outer iteration to the next. XSDRNPM has a special "group banding" option for treating this problem. It involves collecting several groups together into a band and doing one inner for each group in the band while collecting particle balance information. This balance information is then used to solve for one set of flux rebalance factors to apply to each group in the band. Because the band is much wider than an individual group, the scattering that remains within the band is a much larger fraction of the total scattering source for the band. This condition leads to considerably faster convergence from one outer iteration to the next. The group banding option in XSDRNPM is triggered by the seventh entry in the 2$ array. The absolute value of this entry indicates the number of bands to be used. If the number is negative, these bands are only for the thermal groups. Normally there is no need to band together groups other than the thermal groups. An entry of -1 indicates that all the thermal groups will be treated as one band. This mode is one that is used successfully for many problems, but occasionally will cause a problem to not converge. For these problems using two or three bands for the thermal groups has been successful.

The code generates a default banding structure, but this structure can be overridden by inputting a 52$ array.

F3.2.12 BUCKLING CORRECTIONS

XSDRNPM allows "buckling" corrections to be made for the transverse (noncalculated) dimensions in its 1-D slab and cylindrical geometries. Three input parameters-DY, DZ, and BF (5* array)-may be involved.

In the case of the 1-D slab, the height DY and the width DZ can be input. The buckling correction is used to account for leakage in the transverse direction and is treated analogous to an absorption cross section, that is,

$$\text{Tranverse Leakage} = DB^2\psi ,$$

where B is the geometric buckling and is given by

$$B^2 = \left(\frac{\pi}{Y}\right)^2 + \left(\frac{\pi}{Z}\right)^2 ,$$

and Y and Z are the height and width of the slab, respectively, and include extrapolation distances.

Recall that the "extrapolation distance" is defined as the linear extrapolation distance such that if one extrapolated to a zero flux value at this distance from the boundary, the interior flux shape in the body would be correctly represented. The distance can be shown to occur at $0.71\ \lambda_{tr}$, where λ_{tr} is the transport mean free path given by $1/\Sigma_{tr}$. Note that for a slab, there are two extrapolation distances to include (one or either side) for the height and width, such that

$$Y = DY + 1.42\ \lambda_{tr},$$

and

$$Z = DZ + 1.42\ \lambda_{tr}.$$

The 1.42 factor is input in the BF parameter of the 5* array.

In calculating λ_{tr}, a transport cross section, Σ_{tr}, is determined from

$$\Sigma_{tr} = \Sigma_t - \Sigma_{s1}$$

which varies as a function of energy group and zone. The Σ_{s1} term is the within-group term from the P_1 scattering matrix.

In the case of the 1-D cylinder, the procedure is the same as for the slab except that the buckling is determined from

$$B^2 = \left(\frac{\pi}{Y}\right)^2 ,$$

since only one transverse dimension is needed.

The diffusion coefficient in the leakage term is determined from

$$D = \frac{1}{3\Sigma_{tr}} .$$

Note that when comparing with codes or treatments using a fixed value of buckling for every group, a user can force this situation in XSDRNPM by inputting a zero value for BF and DZ and setting DY to determine the required buckling value.

F3.2.13 VOID STREAMING CORRECTION

In real slab and cylindrical geometries, void regions offer streaming paths that are nonexistent in the 1-D cases with quadratures that do not include a vertical angle. A correction for this effect has been suggested by Olsen,[12] who uses an adjustment to the absorption cross section to account for the transverse leakage.

If one considers a slab of height H, the void streaming correction is introduced through an adjustment to the total cross section and is given by

$$\frac{\sqrt{1-\mu_m^2}}{H/2} ,$$

where μ_m is the cosine of the direction.

In the case of a cylinder of height H, the adjustment is

$$\frac{\mu_m}{H/2} .$$

These streaming corrections are very approximate and do not properly account for the fact that the streaming is enhanced near the ends of a void channel; however, they are probably better than the alternative, which is to make no correction at all.

F3.2.14 CROSS-SECTION WEIGHTING

XSDRNPM weights cross sections according to the following four options:

1. "Cell" weighting,

2. "Zone" weighting,

3. "Region" or "vein" weighting, and

4. "Inner cell" weighting

In all cases the "averaged" cross sections are defined in a manner that conserves reaction rates, that is,

$$\bar{\sigma}_G \int_{space} d\vec{r} N_D(\vec{r}) \int_G dE \psi(E,\vec{r}) = \int_{space} d\vec{r} N(\vec{r}) \int_G dE\, \sigma(E,\vec{r})\, \psi(E,\vec{r}) \qquad \text{(F3.2.49)}$$

where

$\bar{\sigma}_G$ ≡ average cross section in group G,

$N_D(\vec{r})$ ≡ number density used in the definition for the weighting option selected,

$\psi(E,\vec{r})$ ≡ weighting spectrum,

$N(\vec{r})$ ≡ real number density as a function of spatial position,

$\sigma(E,\vec{r})$ ≡ cross section in unreduced form.

If we convert to multigroup notation and use W for the weighting spectrum (instead of ψ), Eq. (F3.2.49) becomes

$$\bar{\sigma}_G \sum_{j}^{\substack{applicable\\ spatial\\ regions}} N_D^j \sum_{g \epsilon G} W_g^j = \sum_{j}^{\substack{applicable\\ spatial\\ regions}} N^j \sum_{g \epsilon G} \sigma_g^j W_g^j, \qquad \text{(F3.2.50)}$$

where

$$W_g^j \equiv \int_j d\vec{r} \int_g dE\, \psi(E,\vec{r}) \; . \qquad \text{(F3.2.51)}$$

F3.2.14.1 *"Cell Weighting"*

Cell weighting is consistent with homogenizing the cross sections in a heterogeneous cell. This is the recommended option to prepare cross sections for a real reactor calculation that will be made with a 2- or 3-D model of the reactor. Most of these codes have no provisions for explicitly representing individual fuel elements which are interspersed in a moderator region.

Cell-weighted cross sections are defined in a manner that attempts to preserve the reaction rates which occur in a representative cell from the reactor. In Eq. (F3.2.50) the weighting involves the following substitution:

$$N_D^j \equiv \bar{N} = \frac{\sum_j^{cell} V^j N^j}{\sum_j^{cell} V^j} \qquad \text{(F3.2.52)}$$

where

$V^j \equiv$ volume of zone j.

F3.2.14.2 *"Zone" Weighting*

Zone weighting is the simplest of the three XSDRNPM weighting options. Each zone produces a unique set of cross sections which preserves reaction rates for the zone. In Eq. (F3.2.50), the spatial sum is over the zone considered, and N^j and N_D^j are unity.

Zone weighting is used very frequently, especially for problems whose collapsed cross sections are to be used in a problem whose geometrical and material layout is similar to that in the weighting problem.

F3.2.14.3 *"Region" Weighting*

"Region-" or "vein-" weighted cross sections are weighted "where-the-nuclide-is." In most problems, there are nuclides of secondary importance which do not need a separate "zone-weighted" set for every region in which the nuclide occurs. Examples are the components of stainless steel. Stainless steel is encountered in a variety of locations and flux environments, but generally one set of cross sections for iron, chromium, manganese, nickel, etc., will suffice for most reactor calculations.

In Eq. (F3.2.50), the spatial sum is over all zones which contain the nuclide of interest with

$$N_D^j = N^j. \qquad \text{(F3.2.53)}$$

F3.2.14.4 *"Inner-Cell" Weighting*

For inner-cell weighting, cell weighting is performed over specified innermost regions in the problem. Nuclides outside these regions are not weighted.

This option is generally employed as follows: A "cell" is described in exactly the same manner as for cell weighting (Sect. F3.2.14.1) except that in this case it is surrounded by a homogeneous representation for the remainder of the core and by blankets, reflectors, etc. The flux calculation is made over this complete system, which should have a more realistic treatment of the leakage across the outer boundary of the interior cell. The cell weighting is subsequently made only over the interior cell.

F3.2.14.5 *Multigroup Weighting Equations*

The following are the multigroup forms of the weighting equations used in XSDRNPM:

1. Cell weighting

$$\bar{\sigma}_G \equiv \frac{\sum_j^{IZM} N^j \sum_{g\epsilon G} \sigma_g^j W_g^j}{\bar{N} \sum_j^{IZM} \sum_{g\epsilon G} W_g^j}, \tag{F3.2.54}$$

where

$$\bar{N} \equiv \frac{\sum_j^{IZM} V^j N^j}{\sum_j^{IZM} V^j} \tag{F3.2.55}$$

$$W_g^j \equiv \psi_g^j = \int_j \psi_g(\vec{r}) d\vec{r}\,. \tag{F3.2.56}$$

2. Zone weighting

$$\bar{\sigma}_G^j \equiv \frac{\sum_{g\epsilon G} \sigma_g^j W_g^j}{\sum_{g\epsilon G} W_G^j}. \tag{F3.2.57}$$

3. Region weighting

$$\bar{\sigma}_G \equiv \frac{\sum_j N^j \sum_{g\epsilon G} \sigma_g^j W_g^j}{\sum_j N^j \sum_{g\epsilon G} W_g^j}. \tag{F3.2.58}$$

F3.2.14.6 *Transfer Matrices*

Collapsing transfer matrices is not quite so simple as collapsing cross sections with a single value per group. A group-to-group term in the broad group sense conserves the scattering rate from one group to the other, that is,

$$\bar{N}^* \bar{\sigma}(G \to G') \psi_G \equiv \int_{space} d\vec{r} N(\vec{r}) \int_g dE \psi(E,\vec{r}) \int_{g'} dE' \sigma(E \to E') \tag{F3.2.59}$$

where the asterisk (*) denotes that the number density on the left side of the equation is consistent with the weighting desired. Therefore, the multigroup forms of the weighting equations for components of the transfer matrices are as follows:

1. Cell weighting

$$\bar{\sigma}_{G\to G'} \equiv \frac{\sum_{j}^{IZM} N^j \sum_{g\in G} W_g^j \sum_{g'\in G'} \sigma^j(g\to g')}{\bar{N} \sum_{j}^{IZM} \sum_{g\in G} W_g^j} . \qquad \text{(F3.2.60)}$$

2. Zone weighting

$$\bar{\sigma}^j_{G\to G'} \equiv \frac{\sum_{g\in G} W_g^j \sum_{g'\in G'} \sigma^j(g\to g')}{\sum_{g\in G} W_g^j} . \qquad \text{(F3.2.61)}$$

3. Region weighting

$$\bar{\sigma}_{G\to G'} \equiv \frac{\sum_{j} N^j \sum_{g\in G} W_g^j \sum_{g'\in G'} \sigma^j(g\to g')}{\sum_{j} N^j \sum_{g\in G} W_g^j} . \qquad \text{(F3.2.62)}$$

Theoretically, the higher-than-zero order $\sigma_l(g\to g')$ should be weighted over ψ_l. Since these functions are generally positive-negative, ψ_l weighting does not always work in practice, and XSDRNPM weights the $\sigma_l(g\to g')$, $\ell > 0$, by the scalar flux, which is positive. This procedure gives usable values for most cases.

F3.2.14.7 *Weighting of* $\bar{\nu}$

In weighting parameters such as $\bar{\nu}$, the average number of neutrons produced per fission, one is interested in preserving the fission source; therefore, the weighting is over $\sigma_f\psi$ instead of just ψ. The weighting procedure in XSDRNPM is to calculate $(\overline{\nu\sigma_f})_G$ and $(\bar{\sigma}_f)_G$ using the appropriate choice from Eqs. (F3.2.60), (F3.2.61), or (F3.2.62). Then

$$\bar{\nu}_G = \frac{(\overline{\nu\sigma_f})G}{(\bar{\sigma}_f)G} .$$

F3.2.14.8 *Transport Cross Sections*

Transport cross sections are not as directly related to the physical properties of a material as much as other group-averaged values. Instead of a reaction rate, these numbers must attempt to preserve a "flux

gradient," which not only depends on the cross sections of the material, but is also very strongly influenced by the geometry and the other nuclides in the vicinity of a material.

Two options are provided in XSDRNPM to generate transport cross sections—options based on the "consistent" and "inconsistent" methods for solving the P_l transport equations. These approximations are referred to as the "outscatter" and "inscatter" approximations because of the nature of the equations used.

F3.2.14.8.1 *Outscatter approximation (inconsistent method)*

In the outscatter approximation, the assumption is made that

$$\sigma_{tr}^g = \sigma_t^g - \overline{\mu}^g \sigma_s^g \ . \tag{F3.2.63}$$

When one notes that

$$\overline{\mu}^g \equiv \frac{\sigma_1^g}{3\sigma_0^g} \tag{F3.2.64}$$

and that

$$\sigma_1^g = \sum_{g'} \sigma_1(g \to g') \ , \tag{F3.2.65}$$

where the $\sigma_1(g \to g')$ terms are the P_1 coefficients of the scattering matrix, the origin of the term "outscatter" to designate the approximation is evident.

F3.2.14.8.2 *Inscatter approximation (consistent method)*

In the "consistent" solution of the P_1 point transport equations, it can be shown that

$$\sigma_{tr}(E) = \sigma_t(E) - \frac{1}{3J(E)} \int_0^\infty dE' \, \sigma_1(E' \to E) J(E') \ , \tag{F3.2.66}$$

where $J(E')$ is the current.

If one multiplies the equation by J(E), integrates over group g, and converts to group-averaged form by dividing by $\int_g$ J(E)dE, the following expression is derived:

$$\sigma_{tr}^g = \sigma_t^g - \frac{1}{3J_g} \sum_{g'} \sigma_1(g' \to g) J_{g'} \ . \tag{F3.2.67}$$

This is the "inscatter" approximation. It is consistent because the transport values are explicitly derived from the P_0 and P_1 equations. As a general rule, the transport values from this treatment are "better" than those from the "inconsistent" treatment. However, in some cases (notably hydrogen at lower energies), negative numbers may be calculated which are unusable and the more approximate approach must be used.

F3.2.14.8.3 *Weighting function for transport cross section*

Unfortunately, the matter of choosing a current to use in the "transport" weighting is not simple. In real problems, currents are positive-negative as a function of energy and space. When cross sections are averaged over positive-negative functions, the "law-of-the-mean" no longer holds and the average value can be anything. This unbounded nature leads to real problems in diffusion calculations.

Approximations that inherently guarantee positive currents are generally used in other codes that circumvent the positive-negative problem. For example, in B_n theory the current is given by

$$j \sim \psi,$$

where B and ψ are both positive.

In XSDRNPM, more direct routes that ensure positivity are taken (e.g., one might set $W_g \equiv |W_g|$). This is crudely supported by the following argument:

Consider a 1-D cylindrical calculation. In two dimensions, the current is a vector combination, that is,

$$\vec{J} = \vec{J}_r + \vec{J}_z \,. \tag{F3.2.68}$$

In XSDRNPM, the z direction is treated by using a buckling approximation, that is,

$$\vec{J}_z = B\psi \,. \tag{F3.2.69}$$

In the weighting calculation, we want to weight over the magnitude of the current. In XSDRNPM, the z-current is imaginary, since we are not calculating a z-direction:

$$\vec{J} = \vec{J}_r + \vec{i}B\psi \,. \tag{F3.2.70}$$

The magnitude of a complex quantity is

$$J = \frac{(\vec{J}_r + \vec{i}B\psi)(\vec{J}_r - \vec{i}B\psi)}{\sqrt{(Value_{\vec{r}})^2 + B^2\psi^2}} \,, \tag{F3.2.71}$$

which is always positive.

In a discrete-ordinates calculation, the current is easily obtained since it is the first flux moment. XSDRNPM has the following options for calculating the current:

1. $J_g = \sqrt{(\psi_1^g)^2 + (DB\psi_g)^2}$ (F3.2.72)
2. $J_g = |\psi_1^g|$ (F3.2.73)

3. $J_g = DB^2\psi_g + \int_0^1 d\mu\mu\psi(g,r_{outside},\mu)$ (F3.2.74)

4. $J_g = \frac{\psi_0^g}{\Sigma_t^g}$ (F3.2.75)

5. $J_g = DB\psi_g$ (F3.2.76)

The first option is the recommended option; option 2 treats only the current in the primary direction; option 3 will always be positive and is a weighting over the total leakage from the system. Option 4 is sometimes referred to as a "bootstrap" approximation; option 5 is equivalent to that used in codes that employ B_n theory.

Once the currents are determined, the transport values are determined as set forth in the equations discussed above. For example, consider cell weighting and the "inscatter" approximation,

$$\sigma_{tr}^G = \frac{\sum_j N^j \sum_{g\in G}\left\{J_g\sigma_t^g - \frac{1}{3}\sum_{g'}\sigma_1(g'\to g)J_{g'}\right\}}{\bar{N}\sum_j^{IZM}\sum_{g\in G}J_g} . \quad \text{(F3.2.77)}$$

For cell weighting and the "outscatter" approximation,

$$\sigma_{tr}^G = \frac{\sum_j N^j \sum_{g\in G} J_g\left\{\sigma_t^g - \frac{1}{3}\sum_{g'}\sigma_1(g\to g')\right\}}{\bar{N}\sum_j^{IZM}\sum_{g\in G}J_g} . \quad \text{(F3.2.78)}$$

F3.2.15 ADJOINT CALCULATIONS

XSDRNPM will, upon option, solve the adjoint forms of the 1-D transport equation. Several special procedures apply for the adjoint calculation:

1. The iteration pattern discussed in Sect. F3.2.10 is reversed in energy. The scheme starts with the last (lowest energy) group and proceeds to the first group.

2. The angular quadrature is treated as if it has the reverse directions associated with the angle (e.g., many quadratures start with μ_1 = -1.0. In the adjoint case, this direction is for μ_1 = +1.0).

3. All edits of input fluxes and collapsed cross sections are given in their normal ordering, as opposed to many codes which require their reversal.

Adjoint calculations have many uses and advantages. As opposed to the forward calculation which yields particle density values, the adjoint fluxes are more abstract and can be thought of as particle importances.

Consider, for example, the problem of determining the response of a detector to particles as a function of their energy and direction. Assume the detector is a cylindrical fission chamber that utilizes a foil of ^{235}U in its intervals. The most obvious way to attack this problem is to mock up the detector and make a series of runs that contain sources of identical strength in different angles and energy groups. If an S_8 (24 angles) quadrature were used with 50 energy groups, the 12 × 50 or 600 independent calculations could be used to completely determine the responses. (Here we have taken note that half of the angles will point away from a detector and, hence, produce no response.) The adjoint calculation produces all 600 responses in one run that is no more difficult and time consuming than the typical forward case. In the adjoint case, the detector response (i.e., the fission cross section of ^{235}U would be specified as a source in the foil region and the adjoint fluxes given as a function of energy and angle would be interpreted as the source of neutrons necessary to produce a response of the magnitude to which one required the response to be normalized.

A second important use of adjoint calculations is to establish good biasing factors for Monte Carlo codes. Two recent reports[13,14] discuss the time and accuracy advantages of this approach for shielding and criticality applications and give some real examples as to how to make the calculations.

Perturbation theory uses adjoint and forward fluxes in combination in a manner that determines changes in responses that would arise from changing parameters used in a calculation. One[15] interesting application is to determine the sensitivity of a calculation to changes in one or more cross-section value changes.

F3.2.16 COUPLED NEUTRON-PHOTON CALCULATIONS

In XSDRNPM, it is possible to do a neutron or a photon calculation, depending only on whether the input libraries are for neutrons or gamma rays. It is also possible to do a "coupled neutron-photon" calculation which automatically determines the gamma-ray sources arising from neutron induced interactions in its photon calculation. This calculation, of course, requires an input cross-section library containing three classes of data:

1. neutron cross sections, including neutron-to-neutron transfer matrices,

2. photon production cross sections (i.e., neutron-to-gamma transfer matrices), and

3. gamma-ray cross sections, including gamma-ray-to-gamma-ray transfer matrices.

At present there are no provisions for treating neutrons produced from gamma interactions other than having the user introduce these sources by hand in a sort of iterative procedure, though this reaction is certainly not unknown (cf., deuterium, beryllium-9, and carbon-13). There are several cases where the (γ,n) interaction can be important. If, for example, one looks at neutrons in a water-moderated pool reactor or in a water spent fuel storage tank at large distances from the fuel, the dominant source is from the neutrons produced by the deuterium in the water.

Normally the neutron-photon calculation requires no more input than a single particle run, except in the case where extraneous neutron and/or gamma-ray sources need to be specified. Most output edits will be split into a neutron and a gamma-ray part and will be labeled as such.

F3.2.17 DIFFUSION THEORY OPTION

XSDRNPM can make a 1-D diffusion theory calculation in user-specified energy groups (enter 1's for the appropriate groups of the 46$ array). In this case, the P_1 diffusion equations[16] are solved:

$$A_{I+1}\psi_{1,I+1} - A_I\psi_{1,I} + \sigma_0(\psi_{0,I} + \psi_{0,I}) = S_0^* \tag{F3.2.79}$$

$$\bar{A}_I(\psi_{0,I+1} - \psi_{0,I}) + \sigma_1(\psi_{1,I+1} + \psi_{1,I}) = S_1^*, \tag{F3.2.80}$$

where

$$\psi_1 \equiv P_1 \text{ current}$$

$$\sigma_0 = \left[\Sigma_t - \Sigma_0(g \to g)\right]\frac{V_I}{2.0} \tag{F3.2.81}$$

$$\sigma_1 = \left[3.0\,\Sigma_t - \Sigma_1(g \to g)\right]\frac{V_I}{2.0} \tag{F3.2.82}$$

$S_0^* = P_0$ *sources less the within-group term*

$S_1^* = P_1$ *sources less the within-group term*

$$\bar{A}_I = \frac{A_I + A_{I+1}}{2}$$

V_I = *volume of Ith interval.*

Solving (F3.2.79) for $\psi_{0,I+1}$ and substituting into (F3.2.80), one can write

$$\psi_{1,I+1} = \frac{\bar{A}_I S_0^* - 2\sigma_0\bar{A}_I\psi_{0,I} - \sigma_0 S_1^* + \psi_{1,I}(\sigma_0\sigma_1 + \bar{A}_I A_I)}{\bar{A}_I A_{I+1} - \sigma_0\sigma_1}\,. \tag{F3.2.83}$$

Solving (F3.2.80) for $\psi_{1,I+1}$ and substituting into (F3.2.79), one can write

$$\psi_{0,I+1} = \frac{A_{I+1}S_1^* - 2\sigma_1\bar{A}_I\psi_{1,I} - \sigma_1 S_0^* + \psi_{0,I}(\sigma_0\sigma_1 + \bar{A}_I A_{I+1})}{\bar{A}_I A_{I+1} - \sigma_0\sigma_1} \quad \text{(F3.2.84)}$$

If one assumes

$$\psi_{1,I+1} = P_{I+1}\psi_{0,I+1} - q_{I+1} \quad \text{(F3.2.85)}$$

$$\psi_{1,I} = P_I\psi_{0,I} - q_I \quad \text{(F3.2.86)}$$

and plugs (F3.2.83) and (F3.2.84) into (F3.2.85), solving for $\psi_{1,I}$ yields:

$$\psi_{1,I} = \frac{P_{I+1}(\sigma_0\sigma_1 + \bar{A}_I A_{I+1}) + 2\sigma_0\bar{A}_I}{\sigma_0\sigma_1 + \bar{A}_I A_I + P_{I+1}2\sigma_1\bar{A}_I}\psi_{0,I}$$

$$- \frac{S_0^*(\bar{A}_I + \sigma_1 P_{I+1}) - S_1^*(\sigma_0 + A_{I+1}P_{I+1}) + q_{I+1}(\bar{A}_I A_{I+1} - \sigma_0\sigma_1)}{\sigma_0\sigma_1 + \bar{A}_I A_I + P_{I+1}2\sigma_1\bar{A}_I}, \quad \text{(F3.2.87)}$$

which by inspection and comparison with (F3.2.86) gives expressions for P_I and q_I.

Equations (F3.2.85) and (F3.2.86) can be substituted into (F3.2.79) and solved for $\psi_{0,I+1}$:

$$\psi_{0,I+1} = \frac{\psi_{0,I}(A_I P_I - \sigma_0) + A_{I+1}q_{I+1} - A_I q_I + S_0^*}{A_{I+1}P_{I+1} + \sigma_0}, \quad \text{(F3.2.88)}$$

which is the expression used in XSDRNPM. The procedure solves for arrays of P_I and q_I which are plugged back into the above expression to yield the fluxes.

F3.2.18 INFINITE-MEDIUM THEORY OPTION

It is possible to force the flux calculation in XSDRNPM to use an infinite medium option for any or all energy groups by entering 2's in the appropriate positions in the 46$ array. When a multiregion calculation is requested, the program will first determine spatially averaged cross sections to use in the infinite- medium expression and then place the infinite-medium flux in all spatial regions for use in any subsequent calculations, such as cross-section weighting. All higher flux moments are set to zero.

The balance expression is

$$\left[\Sigma_t^g - \Sigma(g\to g)\right]\psi_g = \frac{1}{k}F_g + S_g, \quad \text{(F3.2.89)}$$

where F_g is the fission source in group g, S_g is the sum of any fixed source and inscattering source, and Σ_t^g and $\Sigma(g \rightarrow g)$ are homogenized total and group-to-group scattering cross sections.

F3.2.19 B_N THEORY OPTION

XSDRNPM can make a B_N calculation in user-specified energy groups (enter 3's for the appropriate groups of the 46$ array). As in the infinite-medium option discussed in Sect. F3.2.18, cross sections in a multiregion system are not homogenized.
The B_N equations[17] can be written

$$\frac{l+1}{2l+1} iB\psi_{l+1} + \frac{l}{2l+1} iB\psi_{l-1} + \Sigma_t \psi_l = S(u)\delta_l^0 + \int du' \Sigma_s^l(u' \rightarrow u)\psi_l(u') \qquad l = 0,1,\ldots,N-1 \tag{F3.2.90}$$

$$\frac{N}{2N+1} iB\psi_{N-1} + \gamma\Sigma_t\psi_N = \int du' \Sigma_s^N(u' \rightarrow u)\psi_N(u') \tag{F3.2.91}$$

$$\psi_{-1} = 0 \tag{F3.2.92}$$

$$\gamma = 1 + \frac{N+1}{2N+1} \frac{iB}{\Sigma_T} \frac{Q_{N+1}(-\Sigma_t/iB)}{Q_N(-\Sigma_t/iB)} \tag{F3.2.93}$$

where δ_l^0 is the Kronecker delta function and Q_N is a Legendre polynomial of the second kind. In multigroup form, the above expressions become:

$$\frac{l+1}{2l+1} iB\psi_{l+1}^g + \frac{l}{2l+1} iB\psi_{l-1}^g + \Sigma_t^g \psi_l^g = S_g\delta_l^0 + \sum_{g'} \Sigma_l(g' \rightarrow g)\psi_l^g \qquad l = 0,1,\ldots N-1 \tag{F3.2.94}$$

$$\frac{N}{2N+1} iB\psi_{N-1}^g + \gamma\Sigma_t^g\psi_N^g = \sum_{g'} \Sigma_N(g' \rightarrow g)\psi_N^g \tag{F3.2.95}$$

$$\psi_{-1}^g = 0 \tag{F3.2.96}$$

In Eqs. (F3.2.90) and (F3.2.94), the S term includes fission, fixed, and scattering source components.

F3.3 SUBROUTINE DESCRIPTIONS

The subroutines particular to the XSDRNPM program are described below in alphabetical order. Subroutines used in XSDRNPM and in other prfgrams in the SCALE system are described in Sect. M2 of the SCALE document.

ACTY - This subroutine computes the pointers needed for computing the reaction rates, clears the arrays that will be used, and calls subroutine RRATE to compute the reaction rates.

ADJNT - This subroutine is used to invert the sources, the flux guess, the white boundary albedos, and the broad-group definition array for an adjoint problem.

BASADR - This subroutine is used to compute the base address array (IBA) pointing to the beginning of each P_l piece of each mixture when the cross sections are stored on random-access storage rather than in memory.

BDYFLX - This subroutine is used to initialize the boundary fluxes after the fluxes have been initialized by a dfffusion calculation using a fission density guess.

BFLUX - BFLUX collapses the fine-group fluxes to broad groups and writes them on the end of the flux tape.

BN - BN calculates the fluxes and moments according to B_n theory. B^2 for the calculation is computed by subroutine SCATSC. BN also estimates a leakage and returns it.

BT - BT computes the pointers for collecting the balance tables, clears the arrays that will be used, writes a head record if the balance table information is being saved, and calls SUMARY to compute and print the balance tables.

CELL - This subroutine computes fluxes using an infinite homogeneous medium approximation.

CFLUX - CFLUX computes and prints the flux disadvantage factors as well as the zone fluxes and currents.

COLAPS - COLAPS is used when a CCCC ISOTXS cross-section interface file is requested to collect the correct 1-D cross sections to be placed on the interface file.

CONVRG - is called at the end of every outer iteration to determine if the code has converged to the answer, and to make a new guess for a search problem.

CURNTS - CURNTS computes the zone fluxes and currents that will be used as weighting functions in producing a weighted cross-section library.

DFLTBN - DFLTBN computes the group banding arrays from the input data.

DIFCOF - DIFCOF initializes the mixture diffusion coefficients to the within group P_0 scattering cross section for the mixture.

DOQ - DOQ computes a default quadrature set for the problem.

DRTRAN - DRTRAN is the control routine for most of the input. It is called after the first data block is read. It performs various initialization functions, computes pointers and storage required for mixing, and prints back the information read in the first data block. Subroutine MIX is then called to mix the cross sections. Subroutine PLSNT is then called to read the rest of the input data, EDIT is called to edit the group boundaries and other input data. Finally, for an adjoint problem, DRTRAN exchanges the neutron and gamma group definitions to account for inverting the group structures.

DT - DT performs the diffusion theory flux calculation required when a fission density guess is supplied, or when flagged in the input.

DWOT - DWOT is a double-precision version of subroutine WOT used to print out the angular fluxes.

EDIT - EDIT is used to compute the inverse velocities from the group boundaries and to print out the energy and lethargy group bounds, the inverse velocities, broad-group definition, calculation by group flags, group banding definition, and right and left albedos. EDIT then adjoints the albedos and calculation by group arrays. It then prints out the mixture by zone array, the order of scattering by zone array, the activity material and reaction type arrays, and the quadrature weights, direction cosines, reflected direction, and weight times cosine arrays. Finally it prints out the constants for converting between angles and moments.

FABCZ - FABCZ evaluates the complex hypergeometric function F(a,b,c,z) using a series expansion. FABCZ is used in calculating the B_n fluxes.

FEWG - FEWG controls the cross-section weighting calculation. It sets up the pointers for the calculation, calls RECRD1 to output the title record on the weighted cross-section tape, sets up the random-access storage to be used in the weighting, call CURNTS to calculate the weighting functions to be used, calls RECRD2 to output the group structure records on the weighted tape, calls WATE to do the cross-section weighting, and calls CFLUX to print the cell-averaged fluxes, the flux disadvantage factors, and the cell-averaged currents.

FILL - FILL is a utility routine used to fill an array with a constant supplied in the calling sequence.

FIND - FIND locates the zeroes of a polynomial by a range-halving technique. It is used in the default quadrature generation process.

FISSRC - FISSRC computes the fission source before each outer iteration. It then computes λ, the ratio of the integral of the new source to the integral of the previous source. Finally, FISSRC scales the fluxes, flux moments, boundary fluxes, and the fission densities by λ.

FIXSRC - FIXSRC computes the total fixed source per group and normalizes the source to the normalization factor input.

FTAPE - FTAPE is used to write the flux guess input in the 33# array onto random-access storage when the fluxes are not held in memory.

FXCEL - FXCEL does outer iteration flux extrapolation when this option has been triggered in the 2$ array. Much of the programming in FXCEL is ad hoc with little testing, and this option is not used by any of the present SCALE procedures.

GEOMF - GEOMF computes the geometry-dependent factors needed in the discrete-ordinates flux calculation. It checks that the input mesh is nonnegative and in increasing order. It modifies the mesh for a search problem.

GETSTS - GETSTS computes the number of sets of weighted cross sections to produce for a given nuclide, and computes an atom density for each set.

HOLLER - HOLLER converts an integer to a bcd number for output on a CCCC interface tape.

INFACE - INFACE controls the flow of converting a weighted cross-section tape to CCCC interface format. The variables for the first two records on the interface file are set up and the records are written. The nuclides on the weighted library are then looped over and those selected for the interface file are put in the correct format and written on a scratch file while the information for the head record for the nuclide is accumulated. The head record is then written on the interface file and the rest of the nuclide data are copied from the scratch file to the interface file.

INNER - INNER is the routine that does the discrete-ordinates angular flux calculation. It uses the current scalar flux and flux moments to calculate the scattering source for the current group. It then loops over the angles, calculating the angular flux at each mesh boundary using a weighted diamond-difference scheme, traversing the mesh in the direction of the current angle. During the sweep, it computes an updated scalar flux and flux moments. When it reaches a system boundary, it saves the new boundary flux.

INVERT - INVERT is used to flip fluxes and flux moments in an adjoint problem back to forward order for printing and writing on the flux tape. If the fluxes are out on random-access storage, they are also rewritten there in forward order for later use in cross-section weighting, activities, and balance tables.

MIX - MIX controls the cross-section mixing. It prints the mixing table and initializes each mixture to zero. It then reads the input cross-section library and mixes the nuclides according to the mixing table. It calls JLL1 to generate a pointer vector for the 2-D cross-section arrays and calls MIXEM to do the actual mixing. After all the mixing is done, it loops back through the mixtures, calling DIFCOF to initialize the diffusion coefficients for each mixture and CMPS to compress out the zeroes from the 2-D arrays and put in the magic words. It calls NCHI to normalize the mixture fission spectrum and to finish generating the mixture diffusion coefficients. During this loop the mixture cross sections are printed if requested by the input. Finally the array pointing to the beginning of each mixture array is calculated.

MIXEM - MIXEM mixes the cross sections from the input library into a mixture. If it is called for 1-D cross sections, it mixes them into the front of the P_0 cross-section array. If the problem is an adjoint problem, the cross sections are mixed in adjoint order.

NCHI - NCHI normalizes the mixed fission spectrum for a mixture, generates a transport cross section, and a mixture diffusion coefficient.

OUTERS - OUTERS is the flow control routine for the flux and search calculation. It calls routines to generate geometry-dependent factors needed in the discrete ordinates flux calculation, to normalize the fixed source, if necessary, to calculate and normalize the fission source, to calculate the scattering source, to calculate the flux according to discrete ordinates, diffusion theory, infinite homogeneous medium, or B_n theory, and to check convergence and compute the search parameter. OUTERS controls the loops over energy groups that define an outer iteration loop. These are actually two nested loops, one over bands and another over groups within a band. The outer iteration monitor table is printed at the end of each outer iteration. This table shows the current value of the eigenvalue and the search parameter as well as the status of the convergence parameters.

OUTPUT - OUTPUT is where the scalar flux is printed, punched, and/or written to an output file when requested. The broad-group fluxes are also printed and saved here if requested.

PHIDIV - PHIDIV divides the weighted cross sections by the weighting flux. Any cross-section truncations to produce an ANISN library are also done here.

PLSNT - PLSNT reads the third, fourth, and fifth data blocks and sets up the storage pointers for the rest of the problem. If not enough storage is available for the problem, data are automatically scheduled to be held on random-access storage until the problem either will fit or no more data are available to be stored on random-access files. PLSNT controls loading the mixed cross sections in memory, adjointing group-dependent arrays if necessary, generating the P_l constants needed in the scattering source and flux calculations, and generating the default discrete-ordinates quadrature set.

PNCNST - PNCNST checks the discrete-ordinates quadrature set and computes the P_n constants that convert between the angular flux and the flux moments.

POSTN - POSTN computes the pointers to the next group of cross sections.

PRTBAL - PRTBAL is used to print the balance tables.

PRTF - PRTF is used to print the scalar fluxes.

Q - Q evaluates the orthogonal polynomials used in generating the discrete-ordinates quadrature set.

QOL - QOL evaluates Legendre polynomials of the second kind for complex arguments. If the absolute value of the argument is less than 1, QOL uses the recursion relation to evaluate the polynomial. If the value is greater than 1, prescriptions involving the hypergeometric function are used. QOL is used when doing the flux calculation using B_n theory.

QRATIO - QRATIO is used in doing the B_n calculation. It evaluates a ratio involving Legendre polynomials of the first and second kind.

QUADWT - QUADWT evaluates the weights corresponding to the roots of the appropriate Legendre polynomial for use in generating the discrete-ordinates quadrature set.

REBALN - REBALN generates flux rebalance factors for an inner iteration.

RECRD1 - RECRD1 computes the values needed for the first record of the weighted cross-section library and then writes the record.

RECRD2 - RECRD2 writes the group boundary records onto the weighted cross-section library. It computes an average inverse velocity and fission spectrum for the problem and writes these on the end of the neutron group boundary record. It then prints these data.

REDF - REDF reads a flux guess from a previously written scalar flux tape.

REPLCE - REPLCE writes the fixed source onto a random-access unit when this is needed because of insufficient memory or because it was requested by the input.

RETRVE - RETRVE retrieves a block of the fixed-source data from random access when needed.

ROOTS - ROOTS solves for the roots of the orthogonal polynomials when generating the discrete-ordinates quadrature set.

RRATE - RRATE calculates the reaction rates specified in the input.

SCALFC - SCALFC calculates the matrix used in upscatter scaling and then calls UPSCAL to solve for the scaling factors.

SCATSC - SCATSC computes the scattering source for a group.

SETUP - SETUP reads the first data block and performs initializations.

SPOUT - SPOUT outputs the library format asked for after a weighting calculation has been done.

STAPE - STAPE writes the input fixed sources to random access if needed.

STORXS - STORXS loads the mixture cross section into memory or onto random access as required.

SUMARY - SUMARY calculates the information printed in the balance tables from the angular and scalar fluxes and the cross sections.

SUMBAL - SUMBAL is used to accumulate data needed in computing the inner iteration scaling factors.

SUMFEW - SUMFEW collapses the balance tables to the few group structure for printing if requested.

TOTAL - TOTAL is used to accumulate the totals over groups and over zones in the balance tables.

TRISOL - TRISOL is used to solve the tridiagonal matrix in B_n theory for the fluxes.

TRNPRT - TRNPRT applies the P_1 term to the transport cross section in the weighting calculation.

TRSCT - TRSCT is used to load the transfer arrays for the CCCC format library from the weighted library.

TR1D - TR1D loads the 1-D cross-section arrays for the CCCC format library from the weighted library.

UPSCAL - UPSCAL solves the upscatter scaling matrix for the scaling factors.

VINVRS - VINVRS computes an inverse velocity for a group assuming a 1/E flux shape above a thermal cutoff and a Maxwellian flux shape below the thermal cutoff.

WAIT - WAIT does the broad-group weighting of the transfer arrays.

WATE - WATE does the flow control of the weighting calculation.

WRTBAL - WRTBAL is used to write the balance table information to an external file.

WRTF - WRTF is used to write the scalar flux tape.

WT1D - WT1D does the broad-group weighting of the reaction cross sections.

XCEL - XCEL is used to accumulate data used in the outer iteration flux acceleration calculation.

XSDRIV - XSDRIV is the overall program flow control routine. It is called after the first data block has been read. It calls DRTRAN to finish reading the data and perform the initialization calculations. OUTERS is then called to do the flux calculation. OUTPUT is called to output the fluxes, BT is called to print the balance tables, FEWG is called to do the cross-section weighting, and SPOUT is called to output the final cross-section library in the requested format.

ZMSH - ZMSH finds the first and last intervals for each zone.

F3.4 FLOW CHART AND OVERLAY STRUCTURE

The following several charts indicate the major program flow paths in XSDRNPM. These charts are not meant to be detailed flow charts and will omit reference to calls to "service routines," etc., but are meant, rather, to give an indication of major processes and major routines associated with theprocesses.

MAIN FLOW

MAIN Program (named XSDRN) – calls SETUP to read the first data block and indirectly calls XSDRIV through ALOCAT. ALOCAT assigns core to XSDRIV which controls the rest of the run.
SETUP assigns some default values, opens several IO buffers and reads the first block of data.
XSDRIV – calls several subroutines which control major processes.
DRTRAN – calculates pointers for various storage blocks, reads the second data block calls MIX to mix macroscopic data, calls PLSNT to read remaining data blocks and to assign other array space and determine many constants needed elsewhere in calculations (see DRTRAN chart).
OUTERS – control module for all flux calculations (see OUTERS chart).
OUTPUT – controls the editing of fine- and broad-group fluxes by interval (see OUTPUT chart).
BT – controls balance table calculation (see BT chart).
ACTY – controls activity table calculation (see ACTY chart).
FEWG – controls cross-section weighting (see FEWG chart).
SPOUT – controls production of ANISN and CCCC libraries (see SPOUT chart).

DRTRAN Calling Chart

MIX	controls mixing of macroscopic cross sections; calls WOT8 to edit the mixing table and other Block 2 data; calls MIXEM for actual mixing; calls DIFCOF to determine diffusion coefficients used in transverse leakage correction; calls CMPS to compress mixed cross sections; calls NCHI to form a mixture-dependent spectrum.
PLSNT	calculates pointers for important arrays; reads data blocks 3, 4, and 5; calls DOQ to calculate S_n constants; calls PNCNST to calculate parameters needed in the S_n flux calculation; may call REDF to read fluxes from a binary flux file; may call STORXS if cross sections are to be stored externally; may call DFLTBN for determining parameters needed in group banding; may call ADJNT to invert some arrays when an adjoint calculation has been requested.

OUTERS Calling Chart

GEOMF –	calculates areas, volumes, and other geometric parameters used in the flux calculation.
FIXSRC –	determines the integrals of the fixed sources by interval.
WOT8 –	called to edit geometrical parameters determined in GEOMF and FIXSRC.
FISSRC –	calculates the fission sources by interval from current flux values.
SCATSC –	calculates the inscattering sources (all moments) from current flux values.
BN –	called if a B_N calculation has been requested.
CELL –	called if an infinite medium calculation has been requested.
DT/BDYFLX –	called if a diffusion theory calculation has been requested. BDYFLX is used to determine boundary values and is only called for the first outer iteration.
INNER –	called if a discrete ordinates calculation is requested.
REBALN –	called to do inner iteration scaling for discrete-ordinates calculation.
XCEL –	writes binary-flux moments tape, if requested.
SCALFC –	generates the upscatter scaling factors.
FXCEL –	outer iteration flux acceleration is done here.
CONVRG –	called to check outer iteration convergence.

Output Calling Chart

INVERT –	called to reorder adjoint fluxes to the normal high-to-low-energy ordering.
PRTF –	called to produce edits of fine-group and/or broad-group fluxes as a function of interval and group.
FFPUN –	called to punch fluxes, if requested.
WRTF –	called to create a "restart" flux moments file, if requested.
BFLUX –	called to determine broad-group fluxes by interval, if requested.

BT Calling Chart

SUMARY	is called to calculate fine- and broad-group balance tables. It also edits angular fluxes on request. SUMFEW is called to determine broad-group parameters.

ACTY Calling Chart

RRATE	is called to calculate the requested activities. WOT and WOT8 are called to edit these values.

FEWG Calling Chart

RECRD1	is used to scan problem input and determine the information necessary to write the first record for the AMPX weighted library.
CURNTS	is called to determine the currents that are used to produce transport cross sections.
RECRD2	is called to determine the energy structure needed for the second record on the working library, along with other group-dependent values such as inverse velocities, χ's, etc.
WATE	is called to weight cross sections. It calls WT1D to weight 1-D data and WAIT to weight-transfer matrices.
CFLUX	is called to calculate volume-averaged fluxes and, hence, disadvantage factors which are edited when a cell weighting is performed.

SPOUT Calling Chart

ANIS is called whenever an ANISN library is to be output.	
	A1DX stuffs 1-D values into appropriate positions in the ANISN matrices.
	SNST stuffs transfer matrix terms into appropriate positions in the ANISN matrices.
	FFPUN may be called to punch ANISN cross sections.
	WOT may be called to edit ANISN cross sections.
INFACE is called whenever a CCCC ISOTXS library is to be output.	
	TR1D is used to procure the 1-D values for the ISOTXS library.
	COLAPS is used to move 1-D data into the structure needed by ISOTXS.
	TRSCT is used to put the total scattering matrix data into the form required for the CCCC ISOTXS file (Ref. 12).

A three-level overlay structure as shown in Fig. F3.4.1 is used at ORNL with XSDRNPM. The structure, along with the routines located in each level, is shown below:

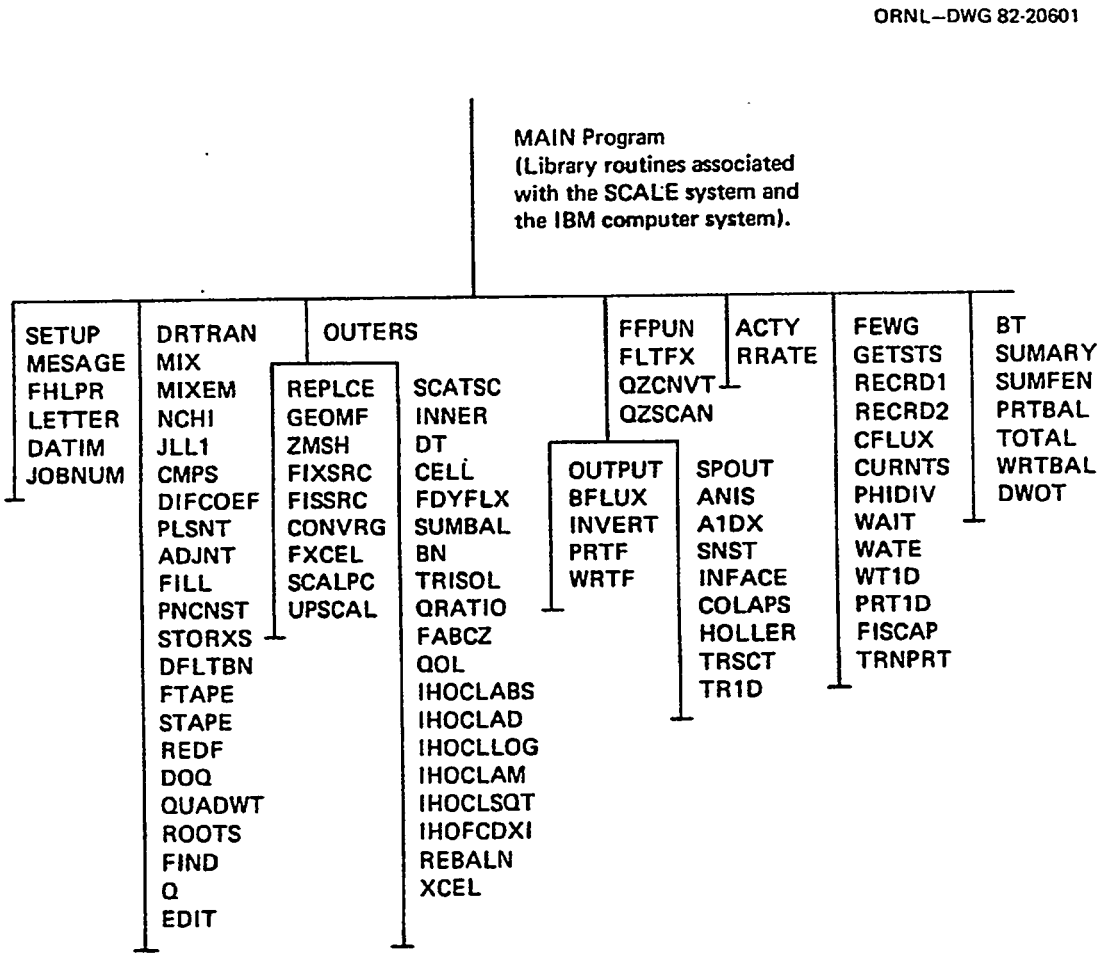


Figure F3.4.1 XSDRNPM overlay structure

F3.5 XSDRNPM INPUT DATA

The input data to XSDRNPM consist of a title card and up to five data blocks, depending on the particular problem. All data in these blocks are entered using the FIDO formats discussed in Sect. M10 of the SCALE manual.

In the description that follows, the quantity in square brackets is the number of items in an array. The quantity in braces is the condition which requires the array to be input. If no condition is specified, an array must be input. Default parameters that are used if an array is not input are shown in parentheses if nonzero.

****

Title Card - Format (20A4)

This is the title card for the problem. It will be used to label the problem output.

Data Block 1

This block contains information to set up various array dimensions and most calculational and editing options. Various convergence criteria and special constants can be input.

0$$ Logical Assignments [11]

1. LPUN- Logical number for punched card output (7).
2. LRSF - Random-access scratch for fluxes (10).
3. LAWL - Input AMPX working library (4).
4. LANC - ANISN binary or CCCC ISOTXS library (20).
5. LOWL - Output weighted library (3).
6. LANG - Angular flux scratch file (16).
7. LSF1 - Sequential scratch space (17).
8. LSF2 - Sequential scratch space (18).
9. LSF3 - Sequential scratch space (19).
10. LRSM - Random-access scratch for macroscopic cross sections (8).
11. LRSX - Random-access scratch for macroscopic cross sections (9).

-1$ Storage Assignment [1]

1. LENG - Maximum length of the storage array (200000)

1$ General Problem Description [15]

1. IGE - problem geometry (1)

   0 - homogeneous (This causes a B_N calculation to be made for all zones-Sect. F3.2.19.)
   1 - slab
   2 - cylinder
   3 - sphere

2. IZM - number of separate material regions or zones. (1)

3. IM - number of spatial intervals in the problem. (1)

4. IBL - the boundary condition at the left-hand boundary of the system. (1)

   0 - vacuum boundary
   1 - reflected boundary
   2 - periodic boundary
   3 - white/albedo boundary

   Boundary conditions are discussed in Sect. F3.2.6.

5. IBR - the boundary condition at the right-hand boundary of the system. (1)

   0 - vacuum boundary
   1 - reflected boundary
   2 - periodic boundary
   3 - white/albedo boundary

6. MXX - the number of compositions used in the problem mock-up.

7. MS - the number of entries in the mixing table which specifies the makeup of the MXX compositions.

8. ISN - the order of angular quadrature to be used. If ISN $>$ 0, XSDRNPM will calculate an angular quadrature for the appropriate geometry. If ISN $<$ 0, the calculation is bypassed, and the user can supply a set in the 42* and 43* arrays.

9. ISCT - the order of scattering. Flux moments will be calculated through this order.

10. IEVT - the type of calculation. (1)

    0 - fixed source
    1 - k calculation
    2 - α calculation (flux is assumed to have an $e^{-\alpha t}$ time variation)
    3 - inoperable in present version
    4 - zone width search
    5 - outer radius search
    6 - buckling search
    7 - direct buckling search

11. IIM - the inner iteration maximum used in an S_n calculation. (10)

12. ICM - the outer iteration maximum. (10)

    After ICM outer iterations, the problem will be forced into the termination phase and the program will continue as if full convergence was attained. A message to this effect is printed.

13. ICLC - theory option. (0)

    0 - use S_n theory always
    N - use alternative theory (diffusion, infinite medium, or B_n for N outer iterations, after which revert back to S_n theory.
    -N - always use alternative theory

14. ITH - forward/adjoint selector. (0)

    0 - solve the forward Boltzmann equation.
    1 - solve the adjoint Boltzmann equation.

15. IFLU - not used. (0)

2$ Editing and Special Options [10]

1. IPRT - fine-group mixture cross-section edits. (-1)
   -2 - no edits
   -1 - edit 1-D cross sections
   0 edit through P_N cross sections.
   N 1-D edits are made, also.

2. ID1 - flux editing options. (0)

IDI	Print Angular Fluxes	Print Scalar Fluxes	Punch[a] Scalar Fluxes
-1	No	No	No
0	No	Yes	No
1	Yes	Yes	No
2	No	Yes	Yes
3	Yes	Yes	Yes

|ID1| > 3 fluxes written on |ID1| in binary format.

[a]The fluxes will be punched in a format suitable for restarting an XSDRNPM calculation.

3. IPBT - balance table edits. (0)

   -1 - none
   0 - make fine-group balance tables
   1 - make fine- and broad-group balance tables

4. ISX - broad-group flux edit as a function of interval. (0) (0/1 = no/yes)

5. ISEN - outer iteration acceleration. Input a zero.

6. IBLN - logical unit on which to output activity file. (0)

7. NBANDS - number of flux rebalance bands.
   < 0, then this is the number of bands in the thermal range.

8. IFSN - If > 0 means no fission source if IEVT=0.

9. NBL - logical unit on which to output balance table file. (0)

10. IDM4 - not used.

    The structure of the "activity" and the "balance table" files are described in Appendix A.

3$ Various Options [12]

1. IFG - cross-section weighting. (0)
   0 - none required
   1 - collapse cross sections

2. IQM - volumetric sources. (0)
   0 - none
   N - N volumetric source spectra will be input in the 31* array

3. IPM - boundary sources. (0)
   0 - none
   N - N boundary source spectra will be input in the 32* array

4. IFN - starting guess. (0)
   0 - flux guess (33# array)
   1 - fission density guess (34# array)
   >2 - unit on which fluxes are stored in a binary format

5. ITMX - maximum time allowed for the flux calculation in minutes. A value of zero specifies that the calculation should not be terminated because of time; otherwise the problem will be forced into the termination phase when ITMX is exceeded. (0) Bear in mind that this is an internal timing check and has no connection with operator or system terminations due to excessive times.

6. IDAT1 - external data storage. If IDAT1 is input as zero, XSDRNPM will automatically select the most efficient means of storing data.

   0 - keep all arrays in core if possible
   1 - store mixture cross sections externally on a direct access device
   2 - store cross sections and fixed sources externally on direct access devices
   3 - store cross sections, fixed sources, and flux moments externally on direct access devices

7. IPN - diffusion coefficient option for transverse leakage corrections. (3)

   0 - determine a transport cross section for each zone using P_0 and P_1 cross sections and, hence, a diffusion coefficient from $1/3\ \Sigma_{tr}$.
   1 - spatially average the diffusion coefficients determined as for the above option and use it for all zones.
   2 - spatially average the transport cross sections for all zones and determine a diffusion coefficient to be used in all zones by taking one over three times this value.
   3 - flux weight the transport cross sections for all zones and determine a diffusion coefficient to be used in all zones by taking one over three times this value.

   Normally, the first option (IPN = 0) is adequate; however, in cases involving regions of low concentration (near void) and, hence, very low transport cross sections, the very large diffusion coefficients lead to nonphysical behavior. In this case, the IPN = 3 option has been demonstrated to operate the best.

8. IDFM - density factors. (0)
   0 - none
   1 - read in density factors in the 38* array

9. IAZ - activity calculation trigger. (0)

   0 - none
   N - calculate the reaction rates by material zone for N different processes specified in the 49$ and 50$ arrays

10. IAI - spatially dependent activity rates. (0)

    0 - none
    1 - calculate reaction rates in each interval for IAZ processes

11. IFCT - thermal upscatter scaling. (0)

    0 - none
    1 - use upscatter scaling for accelerated problem convergence

12. IPVT - parametric eigenvalue search. (0)

    0 - none
    1 - a search calculation will be made for an eigenvalue equal to PV
    2 - an α loss term with α = PV will be added to the transport equation. The α term will depend on the IEVT option selected

4$ Cross-Section Weighting Options [9] {IFG = 1}

1. ICON - type of weighting. (See Sect. F3.2.14.)

   -N - inner cell (with N zones in the cell). Cell weighting is performed over the N innermost regions in the problem. Nuclides outside these regions are not weighted.

   -1 - cell
    0 - zone
    1 - region or vein

2. IGMF - number of energy groups in the collapsed sets.

3. ITP - collapsed output format desired.

   0-19 - cross sections are written only in the AMPX weighted library formats on logical 3. A weighted library is always written when IFG= 1.
   20-29 - output in the CCCC ISOTXS[5] Version 3 format.
   30-39 - output in the ANISN/DOT/MORSE[3] card format.
   40-49 - output in the ANISN/DOT/MORSE[3] binary format on logical 20.

   The various values of ITP (module 10) are used to select the different transport cross-section weighting options mentioned earlier. The options are:

ITP = 0,10,20,... $\sqrt{(\psi_1^g + (DG\psi_g)^2}$
ITP = 1,11,21,... absolute value of current
ITP = 2,12,22,... $DB^2\psi_g$ + outside leakage
ITP = 3,13,23,... ψ/Σ_t^g
ITP = 4,14,24,... DB ψ_g
ITP = other values are reserved for future development and should not be used.

4. IPP - weighted cross section edit option (-1).

   -2 - none
   -1 - edit 1-D data
   0 edit through P_N cross-section arrays.
   N 1-D edits are given.

5. IHTF - total cross-section position in the ANISN *format*[3] or the number of CCCC[5] formatted cross-section sets to be output. (3)

6. NDSF - within-group scattering cross-section position in the ANISN format. (4)

7. NUSF - table length in the ANISN formats. (IGMF + NDSF - 1)

8. IAP - ANISN cross-section edit option or the scattering order to be output on a CCCC ISOTXS file. (-1)

   -1 - ANISN (do not produce edits of ANISN formatted cross sections)
   CCCC (output all orders on the ISOTXS file)

$$\left\{\begin{matrix}0\\N\end{matrix}\right\} - \left(\frac{edit - ANISN}{output - CCCC}\right) \textit{ through the } P_N \textit{ arrays.}$$

9. MSCM - extra "activity" cross sections in ANISN formats. MSCM extra cross-section types are put above the absorption cross-section position in the ANISN formats. The types are specified in the 12$ array.

5* Convergence Criteria and Assorted Constants [12]

1. EPS - overall problem convergence. (10^{-4})

2. PTC - scalar flux convergence. (10^{-4})

3. XNF - normalization factor. (1.0)

When IEVT = 0, the fixed sources are normalized to XNF.
For IEVT > 0, the fission rate is normalized to XNF. (Note that this is different from the original XSDRN program and from the ANISN program which normalized the fission source to XNF.)
When XNF = 0.0, no normalization is made.

4. EV - starting eigenvalue guess for search calculations.

5. EVM - eigenvalue modifier used in a search calculation. The following is a tabulation of recommended values for EV and EVM.

IEVT	Calculation type	EV	EVM
0	Fixed source	0	0
1	k-calculation	0	0
2	Direct α-search	0	0
3	-	-	-
4	Zone width search	0	-0.1
5	Outer radius search	Starting outer radius	-0.1*EV
6	Buckling search	1.0	-0.1
7	Direct buckling search	0.0	0.0

6. BF - buckling factor (1.420892). This parameter is two times the multiplier on the "extrapolation" distance used to determine where a linearly extrapolated line from the asymptotic flux shape would go to zero (E.g., for slabs, the extrapolation distance is $\approx 0.71\lambda_{tr}$ and, hence, BF ≈ 1.42).

7. DY - first transverse dimension in centimeters used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder).

8. DZ - second transverse dimension in centimeters used for a buckling correction (i.e., the width of a slab).

9. VSC - void streaming correction. This is the height of a void streaming path in a cylinder or slab in centimeters. See Sect. F3.2.13.

10. PV - parametric eigenvalue or value for α used when IPVT > 0. When IPVT = I and IEVT > 1, this is the value of k-effective on which the search calculation is to be made (0.0)

11. EQL - eigenvalue convergence for a search. (10^{-3})

12. XNPM - new parameter modifier used in search calculations. (0.75)

T Terminate data block.

****

Data Block 2

This block contains information on the composition of the materials used in the calculation. Also included is an array to select special cross sections for ANISN and an array to identify cross sections written on the CCCC ISOTXS library.

10$ CCCC Transport Cross-Section Selection [IHTF]

This array contains the process identifier for the transport cross section which is to be used on the CCCC ISOTXS library. It is defaulted to 1001 for all nuclides, which selects the "inscatter" or "consistent" transport values. The other option is 1000, which selects the "outscatter" values. Use of this array can become necessary when negative transport values are encountered, such as is the case in some problems with hydrogen in its lower energy groups. This array is input in a one-to-one correspondence with the 16$ and 18 arrays.

12$ Special Cross-Section ENDF/B Identifiers for Inclusion in ANISN Libraries [MSCM]

This option allows the placement of "activity" cross sections in positions 1 through MSCM of ANISN formatted data. The user must ensure that MSCM is consistent with other positional parameters given in the 4$ array. Use ENDF MT numbers to select processes.

The next three arrays (13$, 14$, and 15*) comprise the mixing table in XSDRNPM. The entries in the arrays go together in a one-to-one correspondence to form triplets:

$$\frac{13\$}{M} \quad \frac{14\$}{N} \quad \frac{15*}{X}$$

This command instructs that nuclide N is to be added into mixture M with a concentration (atoms/barn-cm) of X.

13$ Mixture Numbers in Mixing Table [MS]

The values range from 1 to MXX.

14$ Isotope Identifiers in Mixing Table [MS]

A set of data with this identification must be on logical 4, the XSDRNPM working library, though the code will not make checks to ensure this is the case.

15* Isotope Concentrations in Mixing Table [MS]

16$ CCCC Set Selection Identifiers [IHTF]

These are the identifiers for the sets of cross sections on the AMPX weighted library that are to be put on the CCCC ISOTXS library.

18U CCCC Set Identifiers [IHTF]

Cross-section sets on the CCCC ISOTXS library are identified by six-character Hollerith strings (e.g., PU239 could be used for ^{239}Pu, etc.). Since IBM single-precision word-lengths will only hold four characters, this array will require the reading of two times IHTF words. One way to accomplish this is to use the "variable format"—U—option, whereby, the user specifies a two-word format for each six-character string. For example, one can use the following scheme to read these data:

```
18U
((12(A4,A2)))
```

Enter 12 identifiers per card as if they were read in a "12A6" format.

A second way to accomplish reading this array is to use the Hollerith field option, where one could use:

```
18## 6Hxxxxxx 6Hyyyyyy.....
```

where xxxxxx, yyyyyy, etc., are the identifier strings. This array is input in a one-to-one ordering with the 10$ and 16$ arrays.

T Terminate this data block.

Data Block 3 {IEVT = 0}

This block is used to specify fixed sources.

30$ Source Spectrum Number by Interval [IM]
31* Volumetric Source Spectra [IQM*IGM]
32* Surface Source Spectra [IPM*IGM*MM]

Each of the IQM or IPM spectra is specified in the 31* or 32* array and are stacked one after the other in that array. If both volumetric and surface sources are used in the same problem, the surface source number is multiplied by (IQM + I) when entered in the 30$ array.

A volumetric spectrum will consist of IGM (number of energy groups) entries which are the relative **integrated** values of the source in each group.

A surface source is always assumed to be on the right-hand side of a spatial interval. It is input as was the volumetric source, except that each group contains entries for the MM angles in the S_n quadrature chosen for the problem. Note that a surface source is an **integrated** value and is actually a flux condition in the S_n equations.

In the 30$ array, a zero entry specifies that no source is in an interval.

T Terminate this data block.

****

Data Block 4

This data block contains starting guesses for fluxes and fission densities. If fluxes are read from an external device (IFN>3), this data block is omitted. Both arrays in this block are double-precision arrays, which will require the use of the "#" array designator; otherwise the number of entries read into the arrays will be incorrect or may contain nonsensical values for the starting guess.

33# Flux Guess [IM*IGM] {IFN=0}

A guess for the scalar flux is specified in the order: ((FLUX(I,J),I=1,IM),J=1,IGM), where IM is the number of spatial intervals and IGM is the total number of energy groups. For fixed-source problems, without better information, use zeroes. For eigenvalue problems, a nonzero flux guess must be used. The fluxes punched by using the ID1 parameter in the 2$ array can be used here in restart calculations.

34# Fission Density Guess [IM] {IFN=1}

This is a guess at the number of fission neutrons produced in an interval. When IFN = 1, XSDRNPM uses diffusion theory for the first outer iteration, after which it reverts to the normal mode.

T Terminate this data block.

Data Block 5

This block contains the remaining data needed for an XSDRNPM calculation.

35* Interval Boundaries [IM+1] (cm)

This array describes the spatial quadrature into which the problem mock-up is divided. The boundaries are nonnegative and in increasing order. Usually they will start with a zero value, though this is not necessary.

36$ Zone Number for Each Spatial Interval [IM]

Spatial zones should be contiguous.

38* Density Factors by Interval [IM] {IDFM≠0} (1.0)

These factors are used to effect a density variation in a mixture as a function of spatial interval. Zero for a density factor affords a convenient way for mocking a void region.

39$ Mixture Numbers by Zone [IZM]

The mixture that is in a zone is specified here.

40$ Order of Scattering by Zone [IZM] (ISCT)

This is the order, l, of the S_n P_l calculation which is desired in a zone. This number should be no larger than ISCT.

41* Radius Modifiers by Zone [IZM] {IEVT=4}

These parameters specify the relative movement of the width of a zone in a zone width search. A zero indicates that a zone's width is fixed. (See Sect. F3.2.8.)

42* Weights of the Angles in the Discrete-Ordinates Quadrature [MM*]

Input this set if you wish to override those provided by XSDRNPM. See Sects. F3.2.4.3, F3.2.4.4, or F3.2.4.5.

43* Cosines of the Angles in the Discrete-Ordinates Quadrature [MM]

Input this set if you wish to override those provided by XSDRNPM. See Sects. F3.2.4.3, F3.2.4.4, or F3.2.4.5.

46$ Calculational Option by Group [IGM] {ICLC>0}

0 - perform discrete-ordinates calculation for this group.

1 - perform a diffusion calculation for this group for ICLC outer iterations; use discrete-ordinates theory after this.

2 - perform a homogeneous calculation for this group for ICLC outer iterations; then revert back to discrete-ordinates theory.

3 - perform a homogeneous calculation using B_n theory for this group.

---

*MM = ISN + 1 for slabs and spheres,
= ISN*(ISN + 4)/4 for a cylinder.

47* Right-Boundary Albedos by Group [IGM] {IBR=3} (1.0)

A right-boundary albedo is specified for each fine group. The return current is distributed isotropically in angle.

48* Left-Boundary Albedos by Group [IGM] {IBL=3} (1.0)

As for the 47* array but for the left boundary. Note that if IBR or IBL is 3 and the corresponding 47* or 48* array is omitted, XSDRNPM fills the array with 1.0's effecting a boundary with zero net current and with isotropic neutron return.

49$ Material Number for Activities [IAZ] {IAZ≠0}

50$ Process Number for Activities [IAZ] {IAZ≠0}

The 49$ and 50$ arrays provide a means of obtaining the activity (reaction rate) for any process for which cross sections are available in the XSDRNPM calculation. A representative activity table entry is shown below:

ACTIVITY TABLE ENTRY	
49$	50$
M	N

This entry specifies that the activity N for material M be calculated for all parts of the system which contain that material.

If N is <0, a density of 1.0 is used to calculate activities instead of densities in the mixing table. Allowable process identifiers are given in Appendix B.

51$ Broad-Group Numbers [IGM] {IFG≠0}

This array contains the broad-group numbers into which the fine groups are collapsed in a flux-weighting calculation. For example, if the first five fine groups are to be collapsed to the first broad group, the first five entries in the 51$ array are 1, etc. A zero value can be used to ignore (or truncate) a group.

52$ Lower Band Group Numbers [NBANDS]

Group numbers giving the last group in a flux rebalance band. Overrides the default set supplied by XSDRNPM.

F3.5.1 ABBREVIATED XSDRNPM INPUT DESCRIPTION

After several problem setups have been made for XSDRNPM, the user will probably establish a familiarity, such that the more detailed notes given above are not necessary or desirable. Because of this, the following very abbreviated list is given which will, hopefully, benefit many users.

Title Card - (18A4)

DATA BLOCK 1

-1$ - Storage Assignment
1. Maximum Length of Storage Array
0$ - Logical Assignments [11]
1. Punched Cards (7)
2. Direct Access — Fluxes (10)
3. Working Library (4)
4. ANISN or ISOTXS (20)
5. Weighted Library (3)
6. Angular Fluxes (16)
7. Scratch (17)
8. Scratch (18)
9. Scratch (19)
10. Direct Access (8)
11. Direct Access (9)

1$ - General Description [15]
1. IGE - geometry
2. IZM - number of zones
3. IM - number of intervals
4. IBL - left boundary condition
5. IBR - right boundary condition
6. MXX - number of mixtures
7. MS - mixing table length
8. ISN - angular quadrature
9. ISCT - order of scattering
10. IEVT - problem type
11. IIM - inner iteration maximum
12. ICM - outer iteration maximum
13. ICLC - optional theory
14. ITH - forward or adjoint
15. IFLU - zero

2$- Editing and Control Options[IO]
1. Fine-Group-Mixture Edit
2. Fine-Group-Flux Edit
3. Balance Table Edit
4. Broad-Group-Flux Edit
5. Zero
6. Logical Unit for Activities
7. Number of Bands
8. Suppress Fixed-Source Fission
9. Logical Unit for Balance Tables
10. Zero

Title Card - (18A4)

DATA BLOCK 1 (continued)

3$ - Other Options [12]

1. IFG - Weighting Option
2. IQM - Volumetric Sources
3. IPM - Boundary Sources
4. IFN - Starting Guess
5. ITMX - Time Shut-off
6. IDAT1 - Storage Scheme
7. IPN - Diff. Coeff. Option
8. IDFM - Density Factors
9. IAZ - Activities by Zone
10. IAI - Activities by Interval
11. IFCT - Thermal Scaling
12. IPVT - Search on $k \neq 1$

4$ - Weighting Options [9]

1. Type of weighting
2. Number of broad groups
3. Output format
4. Edit option
5. σ_T position or number CCCC
6. σ_{gg} position
7. Table length
8. ANISN edit option
9. Extra cross sections

5* - Floating Point Values [12]

1. EPS - overall convergence
2. PTC - Point flux convergence
3. XNF - normalization
4. EV - starting guess for search
5. EVM - modifier for search
6. BF - buckling factor
7. DY - height
8. DZ - width
9. VSC - void streaming height
10. PV - k for search
11. EQL - search convergence
12. XNPM - search modifier

T Terminate Data Block 1

Title Card - (18A4)

DATA BLOCK 2

10$ CCCC Transport Cross Section Selector [IHTF]
12$ Additional Processes to be put on ANISN Library [MSCM]
13$ Mixture Numbers [MS]
14$ Isotope Identifiers [MS]
15$ Isotope Concentrations [MS]
16$ CCCC Identifiers from Working Library [IHTF]
18U or 18# CCCC Identifiers on ISOTXS [IHTF]

T Terminate the second Data Block.

DATA BLOCK 3

{Required only when IQM or IPM is nonzero.}

30$ Spectrum Number by Interval (IQM > O) or
Right-Hand Interval Boundary (IPM > O) [IM]

31* Volumetric Sources [IQM*IGM]

32* Boundary Sources [IPM*IGM*MM]

T Terminate the third Data Block.

DATA BLOCK 4

{When fluxes are read from an external device-IFN > 3-this block is omitted.}

33# Flux Guess [IM*IGM] {IFN=0}

34# Fission Density Guess [IM] {IFN=1}

T Terminate the fourth Data Block.

Title Card - (18A4)

DATA BLOCK 5

35* Interval Boundaries [IM + 1]
36$ Zone Numbers by Interval [IM]
38* Density Factors [IM]
39$ Mixture Number by Zone [IZM]
40$ Order of Scattering by Zone [IZM]
41* Radius Modifier by Zone [IZM] {IEVT=4}
42* Discrete-Ordinates Cosines [MM]
43* Discrete-Ordinates Weights [MM]
46$ Alternative Theory Selection [IGM] {ICLC>0}
47* Right-Boundary Albedos [IGM]
48* Left-Boundary Albedos [IGM]
49$ Activity Material or Nuclide Numbers [IAZ]
50$ Activity Process Numbers [IAZ] (See Appendix B)
51$ Broad-Group Numbers [IGM] {IFG>0}
52$ Lower-Band-Group Numbers [NBANDS]

T Terminate the fifth Data Block.

F3.6 XSDRNPM INPUT/OUTPUT ASSIGNMENTS

The following logical units can be required in an XSDRNPM calculation.

Logical Unit	Purpose
3	Weighted Library (Produced by XSDRNPM)
4	Working Library (Input)
5	Card Input
6	Standard Output
7	Punch Fluxes or ANISN Libraries
8	Scratch Direct-Access Device for External Cross-Section Storage
9	Scratch Direct-Access Device for Mixing and Weighting Operations
10	Scratch Direct-Access Device for External Flux Moment Storage
16	Angular Fluxes
17	Scratch Device
18	Scratch Device
19	Scratch Device
20	ANISN Binary Libraries or CCCC ISOTXS Interface

F3.7 SAMPLE CASES

In this section, the input and output for a sample case involving a bare, homogeneous 16-cm sphere of a 93% enriched UO_2F_2 solution is presented. The input AMPX working format cross-section library will be read from logical unit 4. The CCCC ISOTXS library will be written on logical unit 20.

The input working library is a temporary 27-group library created by NITAWL-II containing the following nuclides:

Nuclide	Identifier[b]
$^{235}U_{92}$	92235
$^{238}U_{92}$	92238
^{1}H	1001[a]
$^{16}O_{8}$	8016
$^{19}F_{9}$	9019

[a]Water-bound kernel.

[b]These are the identifiers of the sets of data on the library created for the problem.

An S_{16} quadrature is selected with 32 spatial intervals. Activities are requested for $^{235}U_{92}$ absorption and fission and $^{238}U_{92}$ absorption. A collapsed CCCC ISOTXS library is requested in a four-group structure, where the first five groups collapse to a group, the next five to another, etc. The last 12 groups are collapsed to the fourth group.

The input supplied for the case is listed below. If the SCALE DRIVER is not operational, remove the =NITAWL, the END at the end of the NITAWL-II data, the =XSDRN and the END at the end of the XSDRN data. The library created on logical unit 4 by NITAWL-II must be made available to XSDRN. Stacked cases require the SCALE DRIVER or comparable controller.

```
=NITAWL
0$$ 82 E  1$$ A2 5 A8 2 E  1T
2$$ 1001 8016 9019 92235 92238
3**
92235 293. 4Z 3.169E-04 1 1.008 4.21496E+03 1 16.068 4.03814E+02 1 1.
92238 293. 4Z 2.355E-05 1 1.008 5.67153E+04 1 16.448 5.56658E+03 1 1.
 2T
END
=XSDRN
93% UO2F2 SOLUTION SPHERE
1$$ 3 1 32 1 0 1 5 16 1 1 20 10 0 0 0
2$$ A7 -1 E
3$$ 1 A9 3 1 E
4$$ 0 4 20 -1 5 E
5** 2R1.-5 E    1T
13$$          1          1          1          1          1
14$$       1001       8016       9019      92235      92238
15**     6.548-2  3.342-2  6.809-4  3.169-4  2.355-5
16$$       11001      18016      19019     192235     192238
18##    6HH-1     6H0-16    6HF-19    6HU-235   6HU-238
2T
33## F1  4T
35** 31I0.0 16.0
36$$ F1
49$$ 92235 92235 92238
50$$    18    27    27
51$$ 5R1 5R2 5R3 12R4    5T
END
```

The output produced by the case is shown on the following pages.

```
                    93% UO2F2 SOLUTION SPHERE
    1$ ARRAY     15 ENTRIES READ
    2$ ARRAY     10 ENTRIES READ
    3$ ARRAY     12 ENTRIES READ
    4$ ARRAY      9 ENTRIES READ
    5* ARRAY     12 ENTRIES READ
    1T
DIRECT.ACCESS UNIT   9 REQUIRES     2 BLOCKS OF LENGTH  704 FOR CROSS SECTION MIXING.
```

A message is printed as each array and "T" are read.

93% UO2F2 SOLUTION SPHERE

GENERAL PROBLEM DESCRIPTION DATA BLOCK

GENERAL PROBLEM DATA

IGE	1/2/3 = PLANE/CYLINDER/SPHERE	3	ISN	QUADRATURE ORDER	16
IZM	NUMBER OF ZONES	1	ISCT	ORDER OF SCATTERING	1
IM	NUMBER OF SPACIAL INTERVALS	32	IEVT	0/1/2/3/4/5/6=Q/K/ALPHA/C/Z/R/H	1
IBL	0/1/2/3 = VACUUM/REFL/PER/WHITE	1	IIM	INNER ITERATION MAXIMUM	20
IBR	RIGHT BOUNDARY CONDITION	0	ICM	OUTER ITERATION MAXIMUM	10
MXX	NUMBER OF MIXTURES	1	ICLC	-1/0/N--FLAT RES/SN/OPT	0
MS	MIXING TABLE LENGTH	5	ITH	0/1 = FORWARD/ADJOINT	0
IGM	NUMBER OF ENERGY GROUPS	27	IFLU	NOT USED(ALWAYS WGTD)	0
NNG	NUMBER OF NEUTRON GROUPS	27	IPRT	-2/-1/0/N=MIXTURE XSEC PRINT	-1
NGG	NUMBER OF GAMMA GROUPS	0	ID1	0/1/2/3=NO/PRT ND/PCH N/BOTH	0
IFTG	NUMBER OF FIRST THERMAL GROUP	15	IPBT	-1/0/1=NONE/FINE/ALL BAL. PRT	0

1$ and 2$

SPECIAL OPTIONS

IFG	0/1 = NONE/WEIGHTING CALCULATION	1	IPN	0/1/2 DIFF. COEF. PARAM	3
IQM	VOLUMETRIC SOURCES (0/N=NO/YES)	0	IDFM	0/1 = NONE/DENSITY FACTORS 38*	0
IPM	BOUNDARY SOURCES (0/N=NO/YES)	0	IAZ	0/N = NONE/N ACTIVITIES BY ZONE	3
IFN	0/1/2 = INPUT 33*/34*/USE LAST	0	IAI	0/1=NONE/ACTIVITIES BY INTERVAL	1
ITMX	MAXIMUM TIME (MINUTES)	0	IFCT	0/1=NO/YES UPSCATTER SCALING	0
IDT1	0/1/2/3=NO/XSECT/SRCE/FLUX--OUT	0	IPVT	0/1/2=NO/K/ALPHA PARAMETRIC SRCH	0
ISX	BROAD GROUP FLUXES	0	ISEN	OUTER ITERATION ACCELERATION	0
IBLN	ACTIVITY DATA UNIT	0	NBND	BAND REBALN PARAMETER	-1
IBKL	0/1/2 BUCKLING GEOMETRY	0			

3$

WEIGHTING DATA (IFG=1)

ICON	-1/0/1=CELL/ZONE/REGION WEIGHT	0	IHTF	TOTAL XSECT PSN IN BRD GP TABLES	3
IGMF	NUMBER OF BROAD GROUPS	4	NDSF	PSN G-G OR FILE NUMBER	4
ITP	0/10/20/30/40 0/C/E/AC/A	20	NUSF	TABLE LENGTH OR MAX ORDER	7
IPP	-2/-1/0/N=WGTED XSECT PRINT	-1	MSCM	EXTRA 1-D X-SECT POSITIONS	0
IAP	-1/N ANISN XSECT PRINT	-1			

4$

FLOATING POINT PARAMETERS

EPS	OVERALL CONVERGENCE	1.00000E-05	DY	CYL/PLA HT FOR BUCKLING	0.00000E+00
PTC	POINT CONVERGENCE	1.00000E-05	DZ	PLANE DEPTH FOR BUCKLING	0.00000E+00
XNF	NORMALIZATION FACTOR	1.00000E+00	VSC	VOID STREAMING CORRECTION	0.00000E+00
EV	EIGENVALUE GUESS	0.00000E+00	PV	IPVT=1/2--K/ALPHA	0.00000E+00
EVM	EIGENVALUE MODIFIER	0.00000E+00	EQL	EV CHANGE EPS FOR SEARCH	1.00000E-03
BF	BUCKLING FACTOR=1.420892	1.42089E+00	XNPM	NEW PARAM MOD FOR SEARCH	7.50000E-01

5*

THIS CASE WILL REQUIRE 2285 LOCATIONS FOR MIXING
THIS CASE HAS BEEN ALLOCATED 200000 LOCATIONS

93% UO2F2 SOLUTION SPHERE

13$ ARRAY 5 ENTRIES READ

14$ ARRAY 5 ENTRIES READ

15* ARRAY 5 ENTRIES READ

16$ ARRAY 5 ENTRIES READ

18# ARRAY 5 ENTRIES READ

2T

DATA BLOCK 2 (MIXING TABLE, ETC.)

	NUCLIDES ON TAPE	CCCC IDENTIFICATION
1	1001	11001
2	8016	18016
3	9019	19019
4	92235	192235
5	92238	192238

MIXING TABLE

MIXTURE	COMPONENT	ATOM DENSITY	EXTRA XSECT ID'S
1	1001	6.54800E-02	
1	8016	3.34200E-02	
1	9019	6.80900E-04	
1	92235	3.16900E-04	
1	92238	2.35500E-05	

MACROSCOPIC 1-D CROSS SECTIONS FOR MIXTURE 1

	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
1	3.98186E+00	2.29181E+00	1.86203E+00	1.32888E+00	1.03398E+00	9.23993E-01	6.46610E-01	4.67663E-01
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	1.22048E-04	2.59186E-06	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	2.10743E-02	1.88303E-01	2.14891E-01	1.24531E-01	1.66153E-01	1.80466E-01	8.96490E-02	1.38465E-02
5	5.38359E-04	3.80249E-04	4.14960E-04	4.07251E-04	3.93719E-04	3.66327E-04	4.18924E-04	6.19496E-04
6	4.11333E-03	1.63651E-03	4.33148E-04	4.32918E-04	4.31340E-04	4.19969E-04	5.13683E-04	8.53472E-04
7	1.91813E-03	1.12539E-03	1.12249E-03	1.06577E-03	1.00939E-03	9.16363E-04	1.02678E-03	1.50188E-03
8	1.19378E-01	2.00281E-01	2.20619E-01	2.90444E-01	3.94888E-01	4.89474E-01	7.45330E-01	1.16695E+00

	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
1	3.91966E-01	3.74286E-01	3.69895E-01	3.32094E-01	3.22263E-01	3.30321E-01	2.83036E-01	2.73993E-01
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.11940E-04
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
4	1.00557E-03	7.46967E-05	5.87674E-06	4.12832E-07	6.55540E-08	1.29911E-08	1.46814E-09	4.31094E-10
5	1.12134E-03	2.61984E-03	5.92754E-03	1.24383E-02	1.38811E-02	1.14846E-02	4.45848E-03	5.28592E-03
6	1.59564E-03	3.79993E-03	9.22715E-03	2.03477E-02	2.66421E-02	2.36694E-02	9.25736E-03	9.51941E-03
7	2.71332E-03	6.33726E-03	1.43377E-02	3.00859E-02	3.35756E-02	2.77789E-02	1.07841E-02	1.27856E-02
8	1.40534E+00	1.46229E+00	1.47804E+00	1.49269E+00	1.49800E+00	1.49450E+00	1.50898E+00	1.49519E+00

	GRP. 17	GRP. 18	GRP. 19	GRP. 20	GRP. 21	GRP. 22	GRP. 23	GRP. 24
1	2.53087E-01	2.47683E-01	2.63599E-01	2.98456E-01	2.36880E-01	2.34894E-01	2.15446E-01	1.60841E-01
2	4.63866E-03	1.05430E-02	6.43098E-03	2.33693E-03	3.48258E-02	3.68213E-02	3.44241E-02	1.85877E-01
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
4	1.38834E-10	9.94010E-11	1.40532E-10	2.28519E-10	3.34478E-11	3.88071E-11	3.71038E-11	1.00992E-11
5	1.83283E-02	2.87170E-02	1.86151E-02	2.42527E-02	4.50144E-02	5.94729E-02	6.55869E-02	1.02822E-01
6	2.75929E-02	3.77891E-02	2.44016E-02	3.16583E-02	5.94216E-02	8.04568E-02	8.74767E-02	1.33460E-01
7	4.43323E-02	6.94605E-02	4.50260E-02	5.86622E-02	1.08864E-01	1.43852E-01	1.58636E-01	2.48664E-01
8	1.52382E+00	1.54933E+00	1.55011E+00	1.63033E+00	1.79746E+00	1.92875E+00	2.22673E+00	2.75731E+00

	GRP. 25	GRP. 26	GRP. 27
1	1.23719E-01	9.21522E-02	6.43875E-02
2	6.56042E-01	8.37943E-01	2.09073E+00
3	0.00000E+00	0.00000E+00	0.00000E+00
4	2.95638E-12	2.07303E-12	4.94014E-13
5	1.44750E-01	2.16196E-01	4.23502E-01
6	1.86353E-01	2.77621E-01	5.43901E-01
7	3.49957E-01	5.22884E-01	1.02436E+00
8	3.35141E+00	4.27827E+00	5.87849E+00

```
ELAPSED TIME    0.01 MIN.
 12701 LOCATIONS WILL BE USED
 33# ARRAY     864 ENTRIES READ
  4T
 35* ARRAY      33 ENTRIES READ
 36$ ARRAY      32 ENTRIES READ
 49$ ARRAY       3 ENTRIES READ
 50$ ARRAY       3 ENTRIES READ
 51$ ARRAY      27 ENTRIES READ
  5T
```

93% UO2F2 SOLUTION SPHERE
NEUTRON GROUP PARAMETERS

51$

GP	ENERGY BOUNDARIES	LETHARGY BOUNDARIES	MID PT VELOCITIES	BROAD GP NUMBERS
1	2.00000E+07	-6.93147E-01	4.60581E+09	1
2	6.43400E+06	4.40988E-01	2.88737E+09	1
3	3.00000E+06	1.20397E+00	2.12201E+09	1
4	1.85000E+06	1.68740E+00	1.75673E+09	1
5	1.40000E+06	1.96611E+00	1.46535E+09	1
6	9.00000E+05	2.40795E+00	1.06619E+09	2
7	4.00000E+05	3.21888E+00	6.07557E+08	2
8	1.00000E+05	4.60517E+00	2.72415E+08	2
9	1.70000E+04	6.37713E+00	1.13526E+08	2
10	3.00000E+03	8.11173E+00	4.82126E+07	2
11	5.50000E+02	9.80818E+00	2.05946E+07	3
12	1.00000E+02	1.15129E+01	1.01036E+07	3
13	3.00000E+01	1.27169E+01	5.69594E+06	3
14	1.00000E+01	1.38155E+01	3.20957E+06	3
15	3.04999E+00	1.50030E+01	2.10601E+06	3
16	1.77000E+00	1.55471E+01	1.70521E+06	4
17	1.29999E+00	1.58557E+01	1.52544E+06	4
18	1.12999E+00	1.59959E+01	1.42867E+06	4
19	1.00000E+00	1.61181E+01	1.31002E+06	4
20	8.00000E-01	1.63412E+01	9.05898E+05	4
21	4.00000E-01	1.70344E+01	8.13318E+05	4
22	3.25000E-01	1.72420E+01	6.90069E+05	4
23	2.25000E-01	1.76098E+01	4.86933E+05	4
24	9.99998E-02	1.84207E+01	3.57766E+05	4
25	5.00000E-02	1.91138E+01	2.71895E+05	4
26	3.00000E-02	1.96246E+01	1.87283E+05	4
27	1.00000E-02	2.07233E+01	8.88202E+04	4
28	1.00000E-05	2.76310E+01		

From working library

46$ CALC TYPE 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

52$ GROUP BAND 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 15 15 15 15 15 15 15 15 15 15 15

47* RIGHT ALBEDO

48* LEFT ALBEDO

93% UO2F2 SOLUTION SPHERE

39$ 40$ 49$ 50$

	MIXTURE BY ZONE	ORDER P(L) BY ZONE	ACTIVITY TABLE MATL NO.	REACTION
1	1	1	92235	18
2			92235	27
3			92238	27
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
14				
15				
16				
17				

QUADRATURE CONSTANTS

WEIGHTS	DIRECTIONS	REFL DIREC	WT X COS
0	-1.00000E+00	17	0
1.35762E-02	-9.89401E-01	17	-1.34323E-02
3.11268E-02	-9.44575E-01	16	-2.94016E-02
4.75793E-02	-8.65631E-01	15	-4.11861E-02
6.23145E-02	-7.55404E-01	14	-4.70726E-02
7.47980E-02	-6.17876E-01	13	-4.62159E-02
8.45782E-02	-4.58017E-01	12	-3.87382E-02
9.13017E-02	-2.81604E-01	11	-2.57109E-02
9.47253E-02	-9.50125E-02	10	-9.00008E-03
9.47253E-02	9.50125E-02	9	9.00008E-03
9.13017E-02	2.81604E-01	8	2.57109E-02
8.45782E-02	4.58017E-01	7	3.87382E-02
7.47980E-02	6.17876E-01	6	4.62159E-02
6.23145E-02	7.55404E-01	5	4.70726E-02
4.75793E-02	8.65631E-01	4	4.11861E-02
3.11268E-02	9.44575E-01	3	2.94016E-02
1.35762E-02	9.89401E-01	2	1.34323E-02

CONSTANTS FOR P(1) SCATTERING

ANGL	SET 1
1	-1.00000E+00
2	-9.89401E-01
3	-9.44575E-01
4	-8.65631E-01
5	-7.55404E-01
6	-6.17876E-01
7	-4.58017E-01
8	-2.81604E-01
9	-9.50125E-02
10	9.50125E-02
11	2.81604E-01
12	4.58017E-01
13	6.17876E-01
14	7.55404E-01
15	8.65631E-01
16	9.44575E-01
17	9.89401E-01

These are internally calculated.

INT	RADII	MID PTS	ZONE NO.	AREAS	VOLUMES	DENS FACT	RADIUS MOD	SPEC(INT)
1	0	2.50000E-01	1	0	5.23599E-01		0	
2	5.00000E-01	7.50000E-01	1	3.14159E+00	3.66519E+00			
3	1.00000E+00	1.25000E+00	1	1.25664E+01	9.94837E+00			
4	1.50000E+00	1.75000E+00	1	2.82743E+01	1.93731E+01			
5	2.00000E+00	2.25000E+00	1	5.02655E+01	3.19395E+01			
6	2.50000E+00	2.75000E+00	1	7.85398E+01	4.76475E+01			
7	3.00000E+00	3.25000E+00	1	1.13097E+02	6.64970E+01			
8	3.50000E+00	3.75000E+00	1	1.53938E+02	8.84882E+01			
9	4.00000E+00	4.25000E+00	1	2.01062E+02	1.13621E+02			
10	4.50000E+00	4.75000E+00	1	2.54469E+02	1.41895E+02			
11	5.00000E+00	5.25000E+00	1	3.14159E+02	1.73311E+02			
12	5.50000E+00	5.75000E+00	1	3.80133E+02	2.07869E+02			
13	6.00000E+00	6.25000E+00	1	4.52389E+02	2.45568E+02			
14	6.50000E+00	6.75000E+00	1	5.30929E+02	2.86408E+02			
15	7.00000E+00	7.25000E+00	1	6.15752E+02	3.30390E+02			
16	7.50000E+00	7.75000E+00	1	7.06858E+02	3.77515E+02			
17	8.00000E+00	8.25000E+00	1	8.04248E+02	4.27780E+02			
18	8.50000E+00	8.75000E+00	1	9.07920E+02	4.81187E+02			
19	9.00000E+00	9.25000E+00	1	1.01788E+03	5.37736E+02			
20	9.50000E+00	9.75000E+00	1	1.13411E+03	5.97426E+02			
21	1.00000E+01	1.02500E+01	1	1.25664E+03	6.60259E+02			
22	1.05000E+01	1.07500E+01	1	1.38544E+03	7.26230E+02			
23	1.10000E+01	1.12500E+01	1	1.52053E+03	7.95346E+02			
24	1.15000E+01	1.17500E+01	1	1.66190E+03	8.67604E+02			
25	1.20000E+01	1.22500E+01	1	1.80956E+03	9.43001E+02			
26	1.25000E+01	1.27500E+01	1	1.96350E+03	1.02154E+03			
27	1.30000E+01	1.32500E+01	1	2.12372E+03	1.10322E+03			
28	1.35000E+01	1.37500E+01	1	2.29022E+03	1.18805E+03			
29	1.40000E+01	1.42500E+01	1	2.46301E+03	1.27601E+03			
30	1.45000E+01	1.47500E+01	1	2.64208E+03	1.36712E+03			
31	1.50000E+01	1.52500E+01	1	2.82743E+03	1.46136E+03			
32	1.55000E+01	1.57500E+01	1	3.01907E+03	1.55875E+03			
33	1.60000E+01			3.21699E+03				

ELAPSED TIME 0.01 MIN.

per unit height

OUTER ITER	INNER ITERS	1 - BALANCE	EIGENVALUE	1 - SOURCE RATIO	1 - SCATTER RATIO	1 - UPSCAT RATIO	SEARCH PARAMETER	TIME (MIN)
1	376	-4.83652E-05	8.14493E-01	1.86191E-01	1.00000E+00	4.23692E-04	0.00000E+00	0.0842
2	740	2.21282E-05	9.63462E-01	-1.84344E-01	-1.56763E-01	-1.92504E-04	0.00000E+00	0.1525
3	1091	3.75320E-06	9.91945E-01	-2.92398E-02	-2.42518E-02	-3.57911E-05	0.00000E+00	0.2188
4	1431	6.68222E-07	9.99720E-01	-7.78597E-03	-6.43665E-03	-9.67355E-06	0.00000E+00	0.2837
5	1759	-1.46466E-07	1.00197E+00	-2.23912E-03	-1.85018E-03	-2.79391E-06	0.00000E+00	0.3468
6	2021	-1.98853E-07	1.00263E+00	-6.56596E-04	-5.41507E-04	-2.31463E-06	0.00000E+00	0.3973
7	2206	-1.47361E-07	1.00282E+00	-1.92428E-04	-1.59356E-04	-2.56582E-06	0.00000E+00	0.4330
8	2331	-1.42584E-07	1.00288E+00	-5.23736E-05	-4.36650E-05	-2.25660E-06	0.00000E+00	0.4568
9	2385	6.36875E-08	1.00289E+00	-1.24991E-05	-1.02441E-05	-2.86061E-06	0.00000E+00	0.4665

Cumulative

Indicative that Cross Sections Balance

"Ratios" are between outer iterations

GRP TO GRP	INNER ITERS	MFD INT.	MAX. FLUX DIFFERENCE	MSF INT.	MAX. SCALE FACTOR	COARSE MESH
1	1	2	9.27044E-06	17	1.00000E+00	2
2	1	2	8.87304E-06	10	1.00000E+00	4
3	2	20	4.99593E-07	10	1.00000E+00	4
4	2	14	3.99091E-07	7	1.00000E+00	5
5	1	1	8.76353E-06	6	1.00000E+00	6
6	1	2	6.86979E-06	5	1.00000E+00	7
7	1	2	4.79232E-06	3	1.00000E+00	11
8	1	2	3.38121E-06	2	1.00000E+00	16
9	1	2	2.80467E-06	2	1.00000E+00	16
10	1	2	2.29286E-06	2	1.00000E+00	16
11	1	2	1.83695E-06	2	1.00000E+00	16
12	1	2	1.91477E-06	2	1.00000E+00	16
13	1	2	1.77288E-06	2	1.00000E+00	16
14	1	2	1.50133E-06	2	1.00000E+00	16
15	1	1	8.11292E-06	2	9.99996E-01	16
16	1	1	9.07546E-06	2	9.99997E-01	16
17	2	9	3.81129E-08	2	1.00000E+00	16
18	2	11	3.63329E-08	2	1.00000E+00	16
19	1	1	9.20805E-06	2	9.99997E-01	16
20	1	1	6.25789E-06	2	9.99995E-01	16
21	1	1	7.67680E-06	2	9.99997E-01	16
22	1	1	6.07916E-06	2	9.99996E-01	16
23	1	1	1.89325E-06	1	9.99997E-01	32
24	1	32	9.94813E-07	32	9.99998E-01	32
25	1	1	2.32195E-06	1	1.00000E+00	32
26	1	1	3.31851E-06	1	1.00001E+00	32
27	1	1	5.03266E-06	1	1.00001E+00	32

10 2416 -4.77609E-07 1.00290E+00 -1.66156E-06 -2.29634E-06 -8.95275E-07 0.00000E+00 0.4732

FINAL MONITOR LAMBDA 1.00289E+00 PRODUCTION/ABSORPTION 1.81804E+00 ANGULAR FLUX ON 16

Relative change on inners

****** OUTER ITERATION LIMIT REACHED

Particles produced / Particles started

ELAPSED TIME 0.47 MIN.

93% UO2F2 SOLUTION SPHERE

INT.	ZONE NUMBER	RADIUS	INT. MIDPOINT	AREA	VOLUME	PROD DENSITY
1	1	0.00000E+00	2.50000E-01	0.00000E+00	5.23599E-01	7.76532E-05
2	1	5.00000E-01	7.50000E-01	3.14159E+00	3.66519E+00	5.42561E-04
3	1	1.00000E+00	1.25000E+00	1.25664E+01	9.94837E+00	1.46575E-03
4	1	1.50000E+00	1.75000E+00	2.82743E+01	1.93731E+01	2.83361E-03
5	1	2.00000E+00	2.25000E+00	5.02655E+01	3.19395E+01	4.62567E-03
6	1	2.50000E+00	2.75000E+00	7.85398E+01	4.76475E+01	6.81503E-03
7	1	3.00000E+00	3.25000E+00	1.13097E+02	6.64970E+01	9.36852E-03
8	1	3.50000E+00	3.75000E+00	1.53938E+02	8.84882E+01	1.22471E-02
9	1	4.00000E+00	4.25000E+00	2.01062E+02	1.13621E+02	1.54063E-02
10	1	4.50000E+00	4.75000E+00	2.54469E+02	1.41895E+02	1.87964E-02
11	1	5.00000E+00	5.25000E+00	3.14159E+02	1.73311E+02	2.23639E-02
12	1	5.50000E+00	5.75000E+00	3.80133E+02	2.07869E+02	2.60503E-02
13	1	6.00000E+00	6.25000E+00	4.52389E+02	2.45568E+02	2.97951E-02
14	1	6.50000E+00	6.75000E+00	5.30929E+02	2.86408E+02	3.35331E-02
15	1	7.00000E+00	7.25000E+00	6.15752E+02	3.30390E+02	3.72000E-02
16	1	7.50000E+00	7.75000E+00	7.06858E+02	3.77515E+02	4.07258E-02
17	1	8.00000E+00	8.25000E+00	8.04248E+02	4.27780E+02	4.40445E-02
18	1	8.50000E+00	8.75000E+00	9.07920E+02	4.81187E+02	4.70832E-02
19	1	9.00000E+00	9.25000E+00	1.01788E+03	5.37736E+02	4.97781E-02
20	1	9.50000E+00	9.75000E+00	1.13411E+03	5.97426E+02	5.20526E-02
21	1	1.00000E+01	1.02500E+01	1.25664E+03	6.60259E+02	5.38490E-02
22	1	1.05000E+01	1.07500E+01	1.38544E+03	7.26230E+02	5.50844E-02
23	1	1.10000E+01	1.12500E+01	1.52053E+03	7.95346E+02	5.57116E-02
24	1	1.15000E+01	1.17500E+01	1.66190E+03	8.67604E+02	5.56345E-02
25	1	1.20000E+01	1.22500E+01	1.80956E+03	9.43001E+02	5.48203E-02
26	1	1.25000E+01	1.27500E+01	1.96350E+03	1.02154E+03	5.31398E-02
27	1	1.30000E+01	1.32500E+01	2.12372E+03	1.10322E+03	5.05806E-02
28	1	1.35000E+01	1.37500E+01	2.29022E+03	1.18805E+03	4.69219E-02
29	1	1.40000E+01	1.42500E+01	2.46301E+03	1.27601E+03	4.21743E-02
30	1	1.45000E+01	1.47500E+01	2.64208E+03	1.36712E+03	3.58297E-02
31	1	1.50000E+01	1.52500E+01	2.82743E+03	1.46136E+03	2.79462E-02
32	1	1.55000E+01	1.57500E+01	3.01907E+03	1.55875E+03	1.63947E-02
33		1.60000E+01		3.21699E+03		

93% UO2F2 SOLUTION SPHERE

TOTAL FLUX — Units are per unit volume integrated in energy.

INT.	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
1	2.23445E-05	1.70589E-04	1.94755E-04	1.13784E-04	1.58567E-04	2.31962E-04	2.16105E-04	1.58703E-04
2	2.23920E-05	1.70779E-04	1.94934E-04	1.13853E-04	1.58599E-04	2.31969E-04	2.16034E-04	1.58584E-04
3	2.23019E-05	1.70044E-04	1.94088E-04	1.13355E-04	1.57897E-04	2.30940E-04	2.15070E-04	1.57869E-04
4	2.21581E-05	1.68885E-04	1.92756E-04	1.12571E-04	1.56795E-04	2.29323E-04	2.13556E-04	1.56750E-04
5	2.19560E-05	1.67276E-04	1.90909E-04	1.11487E-04	1.55277E-04	2.27099E-04	2.11481E-04	1.55224E-04
6	2.17043E-05	1.65269E-04	1.88607E-04	1.10135E-04	1.53382E-04	2.24321E-04	2.08890E-04	1.53319E-04
7	2.14015E-05	1.62860E-04	1.85842E-04	1.08512E-04	1.51110E-04	2.20992E-04	2.05785E-04	1.51038E-04
8	2.10506E-05	1.60069E-04	1.82641E-04	1.06632E-04	1.48478E-04	2.17135E-04	2.02189E-04	1.48396E-04
9	2.06524E-05	1.56904E-04	1.79010E-04	1.04501E-04	1.45495E-04	2.12764E-04	1.98116E-04	1.45404E-04
10	2.02093E-05	1.53383E-04	1.74972E-04	1.02131E-04	1.42176E-04	2.07903E-04	1.93585E-04	1.42077E-04
11	1.97227E-05	1.49520E-04	1.70540E-04	9.95306E-05	1.38536E-04	2.02570E-04	1.88615E-04	1.38427E-04
12	1.91952E-05	1.45332E-04	1.65737E-04	9.67122E-05	1.34591E-04	1.96791E-04	1.83229E-04	1.34471E-04
13	1.86288E-05	1.40838E-04	1.60583E-04	9.36876E-05	1.30356E-04	1.90589E-04	1.77449E-04	1.30227E-04
14	1.80263E-05	1.36058E-04	1.55100E-04	9.04705E-05	1.25852E-04	1.83992E-04	1.71301E-04	1.25713E-04
15	1.73903E-05	1.31011E-04	1.49312E-04	8.70742E-05	1.21096E-04	1.77027E-04	1.64810E-04	1.20947E-04
16	1.67235E-05	1.25721E-04	1.43245E-04	8.35135E-05	1.16109E-04	1.69723E-04	1.58005E-04	1.15950E-04
17	1.60288E-05	1.20210E-04	1.36922E-04	7.98031E-05	1.10911E-04	1.62113E-04	1.50913E-04	1.10743E-04
18	1.53092E-05	1.14500E-04	1.30372E-04	7.59588E-05	1.05524E-04	1.54227E-04	1.43565E-04	1.05347E-04
19	1.45677E-05	1.08616E-04	1.23622E-04	7.19964E-05	9.99699E-05	1.46097E-04	1.35991E-04	9.97874E-05
20	1.38075E-05	1.02582E-04	1.16698E-04	6.79321E-05	9.42713E-05	1.37758E-04	1.28221E-04	9.40815E-05
21	1.30318E-05	9.64220E-05	1.09631E-04	6.37825E-05	8.84511E-05	1.29244E-04	1.20290E-04	8.82601E-05
22	1.22436E-05	9.01621E-05	1.02447E-04	5.95641E-05	8.25320E-05	1.20588E-04	1.12225E-04	8.23357E-05
23	1.14463E-05	8.38270E-05	9.51756E-05	5.52940E-05	7.65380E-05	1.11827E-04	1.04067E-04	7.63477E-05
24	1.06429E-05	7.74417E-05	8.78457E-05	5.09884E-05	7.04907E-05	1.02993E-04	9.58362E-05	7.02947E-05
25	9.83669E-06	7.10313E-05	8.04857E-05	4.66646E-05	6.44157E-05	9.41258E-05	8.75840E-05	6.42345E-05
26	9.03078E-06	6.46198E-05	7.31228E-05	4.23372E-05	5.83298E-05	8.52462E-05	7.93083E-05	5.81329E-05
27	8.22836E-06	5.82334E-05	6.57871E-05	3.80253E-05	5.22645E-05	7.64108E-05	7.10928E-05	5.20885E-05
28	7.43218E-06	5.18900E-05	5.84972E-05	3.37349E-05	4.62168E-05	6.75966E-05	6.28641E-05	4.59870E-05
29	6.64606E-06	4.56251E-05	5.12959E-05	2.94970E-05	4.02448E-05	5.89166E-05	5.47978E-05	4.00232E-05
30	5.86987E-06	3.94221E-05	4.41558E-05	2.52753E-05	3.42589E-05	5.01757E-05	4.65803E-05	3.38523E-05
31	5.11353E-06	3.33803E-05	3.71982E-05	2.11613E-05	2.84279E-05	4.16860E-05	3.86514E-05	2.79308E-05
32	4.35008E-06	2.72010E-05	3.00326E-05	1.68088E-05	2.20604E-05	3.20895E-05	2.91282E-05	2.04451E-05

INT.	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
1	1.22822E-04	1.13112E-04	1.09012E-04	7.35993E-05	6.50711E-05	6.76244E-05	3.20851E-05	1.85581E-05
2	1.22696E-04	1.12979E-04	1.08877E-04	7.35064E-05	6.49877E-05	6.75374E-05	3.20434E-05	1.85341E-05
3	1.22137E-04	1.12460E-04	1.08374E-04	7.31653E-05	6.46856E-05	6.72230E-05	3.18942E-05	1.84478E-05
4	1.21267E-04	1.11655E-04	1.07596E-04	7.26395E-05	6.42202E-05	6.67389E-05	3.16643E-05	1.83147E-05
5	1.20083E-04	1.10564E-04	1.06542E-04	7.19274E-05	6.35901E-05	6.60836E-05	3.13532E-05	1.81348E-05
6	1.18607E-04	1.09202E-04	1.05229E-04	7.10399E-05	6.28049E-05	6.52670E-05	3.09656E-05	1.79105E-05
7	1.16840E-04	1.07574E-04	1.03658E-04	6.99787E-05	6.18661E-05	6.42907E-05	3.05022E-05	1.76424E-05
8	1.14795E-04	1.05689E-04	1.01840E-04	6.87505E-05	6.07797E-05	6.31609E-05	2.99659E-05	1.73321E-05
9	1.12479E-04	1.03555E-04	9.97819E-05	6.73599E-05	5.95496E-05	6.18818E-05	2.93587E-05	1.69808E-05
10	1.09902E-04	1.01181E-04	9.74928E-05	6.58136E-05	5.81816E-05	6.04593E-05	2.86834E-05	1.65901E-05
11	1.07077E-04	9.85781E-05	9.49826E-05	6.41178E-05	5.66816E-05	5.88993E-05	2.79429E-05	1.61616E-05
12	1.04015E-04	9.57571E-05	9.22622E-05	6.22801E-05	5.50558E-05	5.72086E-05	2.71403E-05	1.56973E-05
13	1.00730E-04	9.27304E-05	8.93434E-05	6.03082E-05	5.33114E-05	5.53943E-05	2.62790E-05	1.51989E-05
14	9.72355E-05	8.95106E-05	8.62380E-05	5.82102E-05	5.14552E-05	5.34636E-05	2.53623E-05	1.46684E-05
15	9.35468E-05	8.61119E-05	8.29600E-05	5.59953E-05	4.94954E-05	5.14248E-05	2.43942E-05	1.41082E-05
16	8.96784E-05	8.25474E-05	7.95216E-05	5.36718E-05	4.74391E-05	4.92854E-05	2.33782E-05	1.35202E-05
17	8.56485E-05	7.88338E-05	7.59388E-05	5.12501E-05	4.52957E-05	4.70547E-05	2.23187E-05	1.29069E-05
18	8.14708E-05	7.49834E-05	7.22231E-05	4.87382E-05	4.30717E-05	4.47396E-05	2.12188E-05	1.22702E-05
19	7.71669E-05	7.10158E-05	6.83930E-05	4.61479E-05	4.07777E-05	4.23508E-05	2.00836E-05	1.16130E-05
20	7.27481E-05	6.69410E-05	6.44575E-05	4.34854E-05	3.84188E-05	3.98933E-05	1.89155E-05	1.09366E-05
21	6.82403E-05	6.27823E-05	6.04385E-05	4.07647E-05	3.60072E-05	3.73798E-05	1.77203E-05	1.02444E-05
22	6.36490E-05	5.85438E-05	5.63391E-05	3.79877E-05	3.35443E-05	3.48115E-05	1.64986E-05	9.53670E-06
23	5.90083E-05	5.42557E-05	5.21869E-05	3.51726E-05	3.10459E-05	3.22044E-05	1.52581E-05	8.81795E-06
24	5.43097E-05	4.99086E-05	4.79723E-05	3.23124E-05	2.85058E-05	2.95526E-05	1.39959E-05	8.08659E-06
25	4.96034E-05	4.55466E-05	4.37354E-05	2.94336E-05	2.59472E-05	2.68799E-05	1.27234E-05	7.34915E-06
26	4.48505E-05	4.11321E-05	3.94403E-05	2.65125E-05	2.33497E-05	2.41663E-05	1.14313E-05	6.60050E-06
27	4.01350E-05	3.67381E-05	3.51543E-05	2.35940E-05	2.07532E-05	2.14534E-05	1.01398E-05	5.85220E-06

28	3.53492E-05	3.22659E-05	3.07868E-05	2.06197E-05	1.81082E-05	1.86924E-05	8.82615E-06	5.09158E-06
29	3.06536E-05	2.78563E-05	2.64708E-05	1.76800E-05	1.54951E-05	1.59675E-05	7.53075E-06	4.34186E-06
30	2.57555E-05	2.32517E-05	2.19763E-05	1.46277E-05	1.27889E-05	1.31544E-05	6.19541E-06	3.57024E-06
31	2.10281E-05	1.87877E-05	1.76256E-05	1.16822E-05	1.01827E-05	1.04530E-05	4.91496E-06	2.83124E-06
32	1.50225E-05	1.32123E-05	1.22955E-05	8.11515E-06	7.04737E-06	7.22890E-06	3.38917E-06	1.95477E-06

INT.	GRP. 17	GRP. 18	GRP. 19	GRP. 20	GRP. 21	GRP. 22	GRP. 23	GRP. 24
1	8.42449E-06	7.34696E-06	1.37004E-05	4.49762E-05	1.37369E-05	2.59336E-05	8.98783E-05	1.26382E-04
2	8.41347E-06	7.33725E-06	1.36821E-05	4.49135E-05	1.37164E-05	2.58926E-05	8.97184E-05	1.26139E-04
3	8.37426E-06	7.30305E-06	1.36184E-05	4.47040E-05	1.36524E-05	2.57717E-05	8.92972E-05	1.25545E-04
4	8.31387E-06	7.25038E-06	1.35201E-05	4.43811E-05	1.35537E-05	2.55852E-05	8.86487E-05	1.24632E-04
5	8.23215E-06	7.17911E-06	1.33872E-05	4.39447E-05	1.34204E-05	2.53335E-05	8.77762E-05	1.23405E-04
6	8.13032E-06	7.09030E-06	1.32216E-05	4.34008E-05	1.32543E-05	2.50198E-05	8.66880E-05	1.21874E-04
7	8.00860E-06	6.98414E-06	1.30236E-05	4.27507E-05	1.30557E-05	2.46449E-05	8.53883E-05	1.20046E-04
8	7.86773E-06	6.86128E-06	1.27944E-05	4.19983E-05	1.28259E-05	2.42109E-05	8.38835E-05	1.17929E-04
9	7.70823E-06	6.72217E-06	1.25350E-05	4.11464E-05	1.25657E-05	2.37196E-05	8.21801E-05	1.15533E-04
10	7.53086E-06	6.56748E-06	1.22465E-05	4.01990E-05	1.22763E-05	2.31732E-05	8.02853E-05	1.12868E-04
11	7.33634E-06	6.39702E-06	1.19301E-05	3.91599E-05	1.19589E-05	2.25739E-05	7.82073E-05	1.09945E-04
12	7.12549E-06	6.21393E-06	1.15871E-05	3.80336E-05	1.16148E-05	2.19242E-05	7.59541E-05	1.06776E-04
13	6.89921E-06	6.01656E-06	1.12190E-05	3.68247E-05	1.12455E-05	2.12269E-05	7.35358E-05	1.03374E-04
14	6.65836E-06	5.80650E-06	1.08272E-05	3.55379E-05	1.08524E-05	2.04845E-05	7.09605E-05	9.97503E-05
15	6.40399E-06	5.58463E-06	1.04134E-05	3.41787E-05	1.04371E-05	1.97004E-05	6.82402E-05	9.59230E-05
16	6.13698E-06	5.35174E-06	9.97899E-06	3.27516E-05	1.00011E-05	1.88770E-05	6.53827E-05	9.19017E-05
17	5.85850E-06	5.10884E-06	9.52590E-06	3.12631E-05	9.54635E-06	1.80181E-05	6.24018E-05	8.77065E-05
18	5.56936E-06	4.85663E-06	9.05541E-06	2.97172E-05	9.07393E-06	1.71258E-05	5.93037E-05	8.33452E-05
19	5.27089E-06	4.59627E-06	8.56970E-06	2.81211E-05	8.58623E-06	1.62045E-05	5.61044E-05	7.88410E-05
20	4.96367E-06	4.32826E-06	8.06969E-06	2.64777E-05	8.08390E-06	1.52555E-05	5.28070E-05	7.41970E-05
21	4.64926E-06	4.05398E-06	7.55793E-06	2.47955E-05	7.56980E-06	1.42842E-05	4.94306E-05	6.94406E-05
22	4.32779E-06	3.77351E-06	7.03460E-06	2.30748E-05	7.04372E-06	1.32900E-05	4.59723E-05	6.45666E-05
23	4.00128E-06	3.48865E-06	6.50305E-06	2.13270E-05	6.50949E-06	1.22802E-05	4.24564E-05	5.96081E-05
24	3.66900E-06	3.19873E-06	5.96201E-06	1.95475E-05	5.96526E-06	1.12512E-05	3.88693E-05	5.45456E-05
25	3.33398E-06	2.90643E-06	5.41653E-06	1.77535E-05	5.41678E-06	1.02137E-05	3.52436E-05	4.94201E-05
26	2.99383E-06	2.60963E-06	4.86266E-06	1.59312E-05	4.85920E-06	9.15815E-06	3.15460E-05	4.41849E-05
27	2.65391E-06	2.31307E-06	4.30924E-06	1.41104E-05	4.30215E-06	8.10231E-06	2.78235E-05	3.88912E-05
28	2.30837E-06	2.01157E-06	3.74666E-06	1.22581E-05	3.73454E-06	7.02436E-06	2.40006E-05	3.34332E-05
29	1.96790E-06	1.71454E-06	3.19240E-06	1.04315E-05	3.17419E-06	5.95601E-06	2.01519E-05	2.78753E-05
30	1.61739E-06	1.40861E-06	2.62156E-06	8.54564E-06	2.59285E-06	4.84231E-06	1.60947E-05	2.19612E-05
31	1.28180E-06	1.11563E-06	2.07456E-06	6.73041E-06	2.02964E-06	3.75173E-06	1.19953E-05	1.58218E-05
32	8.82688E-07	7.66353E-07	1.42244E-06	4.55145E-06	1.34333E-06	2.41927E-06	7.11535E-06	8.58961E-06

INT.	GRP. 25	GRP. 26	GRP. 27
1	8.16129E-05	7.28356E-05	1.53558E-05
2	8.14516E-05	7.26890E-05	1.53247E-05
3	8.10679E-05	7.23471E-05	1.52528E-05
4	8.04777E-05	7.18201E-05	1.51416E-05
5	7.96854E-05	7.11132E-05	1.49926E-05
6	7.86966E-05	7.02307E-05	1.48065E-05
7	7.75163E-05	6.91775E-05	1.45845E-05
8	7.61493E-05	6.79574E-05	1.43273E-05
9	7.46024E-05	6.65771E-05	1.40363E-05
10	7.28811E-05	6.50408E-05	1.37124E-05
11	7.09938E-05	6.33567E-05	1.33574E-05
12	6.89466E-05	6.15296E-05	1.29722E-05
13	6.67499E-05	5.95695E-05	1.25590E-05
14	6.44098E-05	5.74808E-05	1.21186E-05
15	6.19383E-05	5.52756E-05	1.16538E-05
16	5.93410E-05	5.29574E-05	1.11650E-05
17	5.66319E-05	5.05401E-05	1.06556E-05
18	5.38148E-05	4.80258E-05	1.01254E-05
19	5.09059E-05	4.54304E-05	9.57843E-06
20	4.79060E-05	4.27529E-05	9.01390E-06
21	4.48340E-05	4.00118E-05	8.43628E-06
22	4.16851E-05	3.72015E-05	7.84375E-06
23	3.84820E-05	3.43435E-05	7.24156E-06
24	3.52107E-05	3.14239E-05	6.62604E-06
25	3.18983E-05	2.84685E-05	6.00347E-06
26	2.85136E-05	2.54480E-05	5.36676E-06
27	2.50889E-05	2.23924E-05	4.72349E-06
28	2.15551E-05	1.92390E-05	4.05896E-06
29	1.79483E-05	1.60208E-05	3.38259E-06
30	1.40971E-05	1.25820E-05	2.65822E-06
31	1.00493E-05	8.94426E-06	1.90102E-06
32	5.20240E-06	4.44409E-06	9.21890E-07

ELAPSED TIME 0.47 MIN.

FINE GROUP SUMMARY FOR SYSTEM

GRP.	FIX SOURCE	FISS SOURCE	IN SCATTER	SLF SCATTER	OUT SCATTER	ABSORPTION	LEAKAGE	BALANCE
1	0.00000E+00	2.10743E-02	0.00000E+00	8.72682E-03	1.12917E-02	7.13628E-04	9.09009E-03	1.00000E+00
2	0.00000E+00	1.88302E-01	6.45196E-03	1.09615E-01	1.39741E-01	2.05431E-03	5.29585E-02	1.00001E+00
3	0.00000E+00	2.14890E-01	6.64915E-02	8.98616E-02	2.23321E-01	6.16103E-04	5.74390E-02	1.00001E+00
4	0.00000E+00	1.24531E-01	9.00430E-02	5.55798E-02	1.83484E-01	3.56876E-04	3.07260E-02	1.00002E+00
5	0.00000E+00	1.66152E-01	1.58710E-01	1.62245E-01	2.86245E-01	4.90434E-04	3.81203E-02	1.00001E+00
6	0.00000E+00	1.80466E-01	3.10542E-01	3.76028E-01	4.36818E-01	6.98030E-04	5.34816E-02	1.00001E+00
7	0.00000E+00	8.96486E-02	4.92543E-01	6.14923E-01	5.36092E-01	7.93836E-04	4.52972E-02	1.00001E+00
8	0.00000E+00	1.38464E-02	5.77769E-01	7.57578E-01	5.61150E-01	9.65153E-04	2.95377E-02	9.99968E-01
9	0.00000E+00	1.00556E-03	5.58413E-01	6.85310E-01	5.37210E-01	1.38958E-03	2.08708E-02	9.99953E-01
10	0.00000E+00	7.46966E-05	5.36481E-01	6.48073E-01	5.15481E-01	3.03140E-03	1.80862E-02	9.99960E-01
11	0.00000E+00	5.87673E-06	5.19399E-01	6.27957E-01	4.95599E-01	7.05809E-03	1.67714E-02	9.99977E-01
12	0.00000E+00	4.12832E-07	4.28316E-01	3.50697E-01	4.06797E-01	1.04686E-02	1.10494E-02	1.00000E+00
13	0.00000E+00	6.55539E-08	3.94253E-01	2.94579E-01	3.72605E-01	1.20808E-02	9.56983E-03	9.99997E-01
14	0.00000E+00	1.29911E-08	3.95048E-01	3.16964E-01	3.74087E-01	1.11209E-02	9.83605E-03	1.00000E+00
15	0.00000E+00	1.46813E-09	2.32511E-01	1.07715E-01	2.25852E-01	2.05907E-03	4.59336E-03	1.00001E+00
16	0.00000E+00	4.31093E-10	1.48422E-01	4.63802E-02	1.44535E-01	1.22332E-03	2.65999E-03	1.00001E+00
17	0.00000E+00	1.38834E-10	7.61619E-02	1.38649E-02	7.33569E-02	1.60860E-03	1.19432E-03	1.00001E+00
18	0.00000E+00	9.94008E-11	6.77930E-02	1.19711E-02	6.48399E-02	1.92037E-03	1.03155E-03	1.00001E+00
19	0.00000E+00	1.40532E-10	1.15521E-01	3.31878E-02	1.11299E-01	2.31095E-03	1.91019E-03	1.00001E+00
20	0.00000E+00	2.28518E-10	2.82172E-01	2.29531E-01	2.66385E-01	9.82061E-03	5.97060E-03	9.99993E-01
21	0.00000E+00	3.34477E-11	1.22349E-01	4.92717E-02	1.15042E-01	5.61782E-03	1.69133E-03	9.99991E-01
22	0.00000E+00	3.88070E-11	2.10895E-01	1.35229E-01	1.93657E-01	1.43167E-02	2.92575E-03	9.99990E-01
23	0.00000E+00	3.71037E-11	5.48175E-01	8.18182E-01	4.87121E-01	5.33755E-02	7.68647E-03	9.99993E-01
24	0.00000E+00	1.00992E-11	8.73272E-01	1.48219E+00	7.51686E-01	1.13625E-01	7.96259E-03	9.99999E-01
25	0.00000E+00	2.95637E-12	8.32710E-01	1.01034E+00	7.26211E-01	1.02245E-01	4.25691E-03	9.99998E-01
26	0.00000E+00	2.07302E-12	7.39586E-01	1.35694E+00	6.00632E-01	1.35844E-01	3.10983E-03	1.00000E+00
27	0.00000E+00	4.94014E-13	2.72394E-01	3.34723E-01	2.15736E-01	5.61235E-02	5.35680E-04	9.99998E-01
28	0.00000E+00	9.99997E-01	9.05641E+00	1.07277E+01	9.05626E+00	5.51928E-01	4.48362E-01	9.99994E-01

GRP.	RT BDY FLUX	RT LEAKAGE	LFT BDY FLUX	LFT LEAKAGE	N2N RATE	FISS RATE	FLUX*DB**2	TOTAL FLUX
1	3.95664E-06	9.09009E-03	2.22547E-05	0.00000E+00	2.11743E-05	9.34009E-05	0.00000E+00	1.73492E-01
2	2.39652E-05	5.29585E-02	1.70073E-04	0.00000E+00	3.25355E-06	4.77324E-04	0.00000E+00	1.25530E+00
3	2.62524E-05	5.74390E-02	1.94205E-04	0.00000E+00	0.00000E+00	5.90232E-04	0.00000E+00	1.42238E+00
4	1.44448E-05	3.07260E-02	1.13499E-04	0.00000E+00	0.00000E+00	3.35717E-04	0.00000E+00	8.24352E-01
5	1.84820E-05	3.81203E-02	1.58239E-04	0.00000E+00	0.00000E+00	4.47659E-04	0.00000E+00	1.13700E+00
6	2.64968E-05	5.34816E-02	2.31530E-04	0.00000E+00	0.00000E+00	6.08872E-04	0.00000E+00	1.66210E+00
7	2.32084E-05	4.52972E-02	2.15790E-04	0.00000E+00	0.00000E+00	6.47397E-04	0.00000E+00	1.54538E+00
8	1.55159E-05	2.95377E-02	1.58543E-04	0.00000E+00	0.00000E+00	7.00559E-04	0.00000E+00	1.13085E+00
9	1.10410E-05	2.08708E-02	1.22731E-04	0.00000E+00	0.00000E+00	9.76528E-04	0.00000E+00	8.70861E-01
10	9.56833E-06	1.80862E-02	1.13042E-04	0.00000E+00	0.00000E+00	2.08998E-03	0.00000E+00	7.97751E-01
11	8.85765E-06	1.67714E-02	1.08951E-04	0.00000E+00	0.00000E+00	4.53413E-03	0.00000E+00	7.64927E-01
12	5.82974E-06	1.10494E-02	7.35598E-05	0.00000E+00	0.00000E+00	6.39929E-03	0.00000E+00	5.14484E-01
13	5.04710E-06	9.56983E-03	6.50373E-05	0.00000E+00	0.00000E+00	6.29434E-03	0.00000E+00	4.53447E-01
14	5.18146E-06	9.83605E-03	6.75893E-05	0.00000E+00	0.00000E+00	5.39592E-03	0.00000E+00	4.69841E-01
15	2.42068E-06	4.59336E-03	3.20690E-05	0.00000E+00	0.00000E+00	9.91676E-04	0.00000E+00	2.22425E-01
16	1.40022E-06	2.65999E-03	1.85486E-05	0.00000E+00	0.00000E+00	6.79285E-04	0.00000E+00	1.28508E-01
17	6.29451E-07	1.19432E-03	8.42029E-06	0.00000E+00	0.00000E+00	1.06849E-03	0.00000E+00	5.82975E-02
18	5.44237E-07	1.03155E-03	7.34342E-06	0.00000E+00	0.00000E+00	1.45934E-03	0.00000E+00	5.08182E-02
19	1.00805E-06	1.91019E-03	1.36939E-05	0.00000E+00	0.00000E+00	1.76293E-03	0.00000E+00	9.47044E-02
20	3.16268E-06	5.97060E-03	4.49585E-05	0.00000E+00	0.00000E+00	7.52334E-03	0.00000E+00	3.10207E-01
21	9.01895E-07	1.69133E-03	1.37330E-05	0.00000E+00	0.00000E+00	4.25575E-03	0.00000E+00	9.45419E-02
22	1.56612E-06	2.92575E-03	2.59290E-05	0.00000E+00	0.00000E+00	1.05827E-02	0.00000E+00	1.77942E-01
23	4.12039E-06	7.68647E-03	8.98806E-05	0.00000E+00	0.00000E+00	4.00190E-02	0.00000E+00	6.10168E-01
24	4.27439E-06	7.96259E-03	1.26403E-04	0.00000E+00	0.00000E+00	8.75399E-02	0.00000E+00	8.51379E-01
25	2.29732E-06	4.25691E-03	8.16310E-05	0.00000E+00	0.00000E+00	7.94191E-02	0.00000E+00	5.48663E-01
26	1.69200E-06	3.10983E-03	7.28533E-05	0.00000E+00	0.00000E+00	1.05788E-01	0.00000E+00	4.89315E-01
27	2.96027E-07	5.35680E-04	1.53589E-05	0.00000E+00	0.00000E+00	4.36998E-02	0.00000E+00	1.03187E-01
28	2.22160E-04	4.48357E-01	2.36582E-03	0.00000E+00	2.44278E-05	4.14381E-01	0.00000E+00	1.67623E+01

Volume Integrated

ELAPSED TIME 0.48 MIN.

93% UO2F2 SOLUTION SPHERE

ACTIVITY TABLE

	MATERIAL	REACTION
1	92235	18
2	92235	27
3	92238	27

U^{235} fissions
U^{235} absorptions
U^{238} absorptions

ACTIVITIES BY ZONE

ZONE	ACT. 1	ACT. 2	ACT. 3
1	4.14329E-01	4.97117E-01	2.71197E-03
2	4.14329E-01	4.97117E-01	2.71197E-03

Volume integrated

ZONE 2 HAS SYSTEM TOTALS

ACTIVITIES BY INTERVAL

INT.	ACT. 1	ACT. 2	ACT. 3
1	6.12756E-05	7.34669E-05	3.89338E-07
2	6.11615E-05	7.33309E-05	3.88848E-07
3	6.08743E-05	7.29867E-05	3.87043E-07
4	6.04318E-05	7.24564E-05	3.84260E-07
5	5.98373E-05	7.17436E-05	3.80491E-07
6	5.90954E-05	7.08541E-05	3.75795E-07
7	5.82095E-05	6.97920E-05	3.70179E-07
8	5.71836E-05	6.85621E-05	3.63680E-07
9	5.60227E-05	6.71702E-05	3.56321E-07
10	5.47308E-05	6.56215E-05	3.48137E-07
11	5.33145E-05	6.39234E-05	3.39163E-07
12	5.17783E-05	6.20817E-05	3.29436E-07
13	5.01299E-05	6.01055E-05	3.18999E-07
14	4.83740E-05	5.80005E-05	3.07892E-07
15	4.65199E-05	5.57777E-05	2.96165E-07
16	4.45715E-05	5.34420E-05	2.83861E-07
17	4.25396E-05	5.10062E-05	2.71034E-07
18	4.04271E-05	4.84739E-05	2.57723E-07
19	3.82463E-05	4.58598E-05	2.43993E-07
20	3.59979E-05	4.31647E-05	2.29874E-07
21	3.36962E-05	4.04059E-05	2.15438E-07
22	3.13379E-05	3.75795E-05	2.00694E-07
23	2.89402E-05	3.47061E-05	1.85737E-07
24	2.64930E-05	3.17736E-05	1.70533E-07
25	2.40179E-05	2.88078E-05	1.55217E-07
26	2.14913E-05	2.57809E-05	1.39671E-07
27	1.89414E-05	2.27267E-05	1.24130E-07
28	1.63162E-05	1.95831E-05	1.08301E-07
29	1.36538E-05	1.63967E-05	9.26462E-08
30	1.08258E-05	1.30141E-05	7.64254E-08
31	7.89794E-06	9.51717E-06	6.07340E-08
32	4.34139E-06	5.26966E-06	4.18834E-08

per unit volume

ELAPSED TIME 0.48 MIN.

DIRECT ACCESS UNIT 9 REQUIRES 35 BLOCKS OF LENGTH 260 FOR CROSS SECTION WEIGHTING.

TRANSPORT CROSS SECTION WEIGHTING FUNCTION

ZONE	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
1	3.40541E-06	2.03665E-05	2.20473E-05	1.17243E-05	1.42513E-05	1.95246E-05	1.56098E-05	9.32290E-06
2	3.40541E-06	2.03665E-05	2.20473E-05	1.17243E-05	1.42513E-05	1.95246E-05	1.56098E-05	9.32290E-06

ZONE	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
1	6.17704E-06	5.22127E-06	4.85935E-06	3.22972E-06	2.81457E-06	2.93124E-06	1.37197E-06	8.01753E-07
2	6.17704E-06	5.22127E-06	4.85935E-06	3.22972E-06	2.81457E-06	2.93124E-06	1.37197E-06	8.01753E-07

ZONE	GRP. 17	GRP. 18	GRP. 19	GRP. 20	GRP. 21	GRP. 22	GRP. 23	GRP. 24
1	3.58243E-07	3.07778E-07	5.68673E-07	1.72664E-06	4.62941E-07	7.61098E-07	1.84293E-06	1.76129E-06
2	3.58243E-07	3.07778E-07	5.68673E-07	1.72664E-06	4.62941E-07	7.61098E-07	1.84293E-06	1.76129E-06

ZONE	GRP. 25	GRP. 26	GRP. 27	GRP. 28
1	8.59895E-07	5.46716E-07	7.44474E-08	1.52910E-04
2	8.59895E-07	5.46716E-07	7.44474E-08	1.52910E-04

These values are normally currents.

BROAD GROUP PARAMETERS

GRP	UPPER ENERGY	MID ENERGY	VELOCITY	FISS SPEC
1	2.0000E+07	2.7921E+06	2.0154E+09	7.1495E-01
2	9.0000E+05	2.2644E+05	1.8499E+08	2.8504E-01
3	5.5000E+02	9.0113E+01	5.7786E+06	6.3696E-06
4	1.7700E+00	2.3978E-01	3.3945E+05	1.1634E-09
5	1.0000E-05			

93% UO2F2 SOLUTION SPHERE
HYDROGEN ENDF/B-IV MAT 1269/THRM1002 UPDATED 10/12/89
ZONE WEIGHTED CROSS SECTIONS FOR XSDRN MATERIAL 11001

XSEC ID GRP.	1 (σ_T)	2 ($\sigma_{elastic}$)	27 (σ_a)	101 (σ_c)	102 ($\sigma_{n\gamma}$)	1099 (Flux)	1000 (σ_{tr})	1001
1	2.83703E+00	2.83700E+00	3.49471E-05	3.49471E-05	3.49471E-05	2.80495E-04	9.15823E-01	1.63093E+00
2	1.24471E+01	1.24468E+01	3.56161E-04	3.56161E-04	3.56161E-04	3.50111E-04	3.75227E+00	3.33428E+00
3	2.04879E+01	2.04753E+01	1.26536E-02	1.26553E-02	1.26553E-02	1.41347E-04	6.93026E+00	6.45378E+00
4	3.83916E+01	3.81844E+01	2.07157E-01	2.07668E-01	2.07668E-01	2.05029E-04	2.02633E+01	1.82031E+01

outscatter approx.

inscatter approx.

93% UO2F2 SOLUTION SPHERE
OXYGEN-16 ENDF/B-IV MAT 1276 UPDATED 10/12/89
ZONE WEIGHTED CROSS SECTIONS FOR XSDRN MATERIAL 18016

XSEC ID GRP.	1	2	4 $\sigma_{inelastic}$	101	102	103 $\sigma_{n,p}$	104 $\sigma_{n,d}$
1	2.23707E+00	2.21816E+00	5.82027E-03	1.30935E-02	1.30935E-02	1.96349E-08	4.60067E-05	8.67681E-06
2	3.66070E+00	3.66070E+00	0.00000E+00	2.09747E-07	2.09747E-07	2.09747E-07	0.00000E+00	0.00000E+00
3	3.74792E+00	3.74792E+00	0.00000E+00	6.75895E-06	6.75895E-06	6.75895E-06	0.00000E+00	0.00000E+00
4	3.82685E+00	3.82674E+00	0.00000E+00	1.11099E-04	1.11099E-04	1.11099E-04	0.00000E+00	0.00000E+00

XSEC ID GRP.	107 $\sigma_{n,\alpha}$	1099	51	52	53	54	55	56
1	1.30388E-02	2.80495E-04	2.01769E-03	2.79345E-03	4.17982E-04	3.74750E-04	1.05705E-04	2.75704E-05
2	0.00000E+00	3.50111E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	0.00000E+00	1.41347E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	0.00000E+00	2.05029E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

XSEC ID GRP.	57	58	59	60	61	62	63	64
1	2.70482E-05	1.36722E-05	1.57681E-06	6.54012E-06	5.49071E-06	1.10661E-06	5.72712E-06	3.25827E-06
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
GRPS	3 THRU	4 ARE THE SAME AS ABOVE						

XSEC ID GRP.	65	66	67	68	69	70	71	72
1	4.52046E-06	3.75095E-07	7.15077E-07	1.07991E-06	1.35362E-07	7.33329E-07	2.12736E-06	1.79768E-06
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
GRPS	3 THRU	4 ARE THE SAME AS ABOVE						

XSEC ID GRP.	73	74	75	76	77	78	79	80
1	1.53759E-06	1.29724E-06	1.07025E-06	8.67748E-07	6.92005E-07	5.40562E-07	4.14983E-07	3.10965E-07
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
GRPS	3 THRU	4 ARE THE SAME AS ABOVE						

XSEC ID GRP.	81	82	83	84	85	86	87	88
1	2.31568E-07	1.66856E-07	1.18261E-07	8.16742E-08	5.34034E-08	3.30114E-08	1.75543E-08	7.33272E-09
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
GRPS	3 THRU	4 ARE THE SAME AS ABOVE						

XSEC ID GRP.	89	1007	1000	1001
1	1.75853E-09	0.00000E+00	1.88695E+00	1.77249E+00
2	0.00000E+00	0.00000E+00	3.49883E+00	3.63972E+00
3	0.00000E+00	3.43776E-01	3.62515E+00	3.62770E+00
4	0.00000E+00	3.82675E+00	3.62484E+00	3.65555E+00

MT's 51-90 are used for discrete level inelastic scattering.

93% UO2F2 SOLUTION SPHERE
FLUORINE ENDF/B-IV MAT 1277 UPDATED 10/12/89
ZONE WEIGHTED CROSS SECTIONS FOR XSDRN MATERIAL 19019

XSEC ID GRP.	1	2	4	16 ($\sigma_{n,2n}$)	22 ($\sigma_{n,n\alpha}$)	28 ($\sigma_{n,np}$)	27	101
1	2.64253E+00	1.69238E+00	9.26095E-01	2.14045E-05	3.81531E-04	1.08947E-05	2.36476E-02	2.36476E-02
2	4.56778E+00	3.61190E+00	9.54918E-01	0.00000E+00	0.00000E+00	0.00000E+00	9.51855E-04	9.51855E-04
3	3.94430E+00	3.94393E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.63643E-04	3.63643E-04
4	4.07575E+00	4.06982E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.92919E-03	5.92919E-03

XSEC ID GRP.	102	103	104	105 ($\sigma_{n,t}$)	107	1099	51	52
1	5.85762E-05	1.82743E-03	9.82732E-05	2.08065E-05	2.16425E-02	2.80495E-04	2.58527E-01	4.39273E-01
2	9.51855E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.50111E-04	5.06315E-01	4.46579E-01
3	3.63643E-04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.41347E-04	0.00000E+00	0.00000E+00
4	5.92919E-03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.05029E-04	0.00000E+00	0.00000E+00

XSEC ID GRP.	53	54	55	56	57	58	59	60
1	5.83659E-02	5.86241E-02	8.02510E-02	4.95446E-03	3.40513E-03	2.26254E-03	1.31864E-03	1.94327E-03
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
GRPS	3 THRU	4 ARE THE SAME AS ABOVE						

XSEC ID GRP.	61	62	63	64	65	66	67	68
1	2.45530E-03	1.60179E-03	4.69187E-05	1.45143E-03	9.14360E-04	3.98734E-04	9.54259E-04	6.03718E-04
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
GRPS	3 THRU	4 ARE THE SAME AS ABOVE						

XSEC ID GRP.	69	70	71	91	1007	1000	1001
1	5.81646E-04	6.47808E-04	8.81557E-04	5.12538E-03	0.00000E+00	2.13148E+00	2.12731E+00
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.15170E+00	4.14874E+00
3	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.66635E-01	3.80390E+00	3.81598E+00
4	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.06982E+00	3.89043E+00	3.91838E+00

Continuum inelastic scattering

93% UO2F2 SOLUTION SPHERE
URANIUM-235 ENDF/B-IV MAT 1261 UPDATED 10/12/89
ZONE WEIGHTED CROSS SECTIONS FOR XSDRN MATERIAL 192235

XSEC ID GRP.	1	2	4	16	18	17	27	101
1	7.23513E+00	4.29809E+00	1.62243E+00	1.36994E-02	1.24410E+00	1.31248E-05	1.30088E+00	5.67792E-02
2	1.27012E+01	8.67271E+00	5.33446E-01	0.00000E+00	2.63881E+00	0.00000E+00	3.49507E+00	8.56251E-01
3	6.19767E+01	1.20879E+01	0.00000E+00	0.00000E+00	3.07283E+01	0.00000E+00	4.98889E+01	1.91605E+01
4	4.18644E+02	1.48424E+01	0.00000E+00	0.00000E+00	3.44285E+02	0.00000E+00	4.03801E+02	5.95167E+01

XSEC ID GRP.	102	452	1099	1018	51	52	53	54
1	5.67792E-02	2.75928E+00	2.80495E-04	7.14959E-01	0.00000E+00	8.38629E-02	2.27007E-02	2.16893E-02
2	8.56251E-01	2.43399E+00	3.50111E-04	2.85048E-01	1.88998E-02	1.82039E-01	6.96493E-02	2.41418E-02
3	1.91605E+01	2.41881E+00	1.41347E-04	6.36974E-06	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	5.95167E+01	2.41839E+00	2.05029E-04	1.16339E-09	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

XSEC ID GRP.	55	56	57	58	59	60	61	62
1	2.16834E-02	2.26955E-02	2.18111E-02	2.18111E-02	1.10099E-01	6.18704E-01	3.34978E-03	1.34665E-03
2	2.29951E-02	6.47606E-02	3.22539E-02	2.87727E-02	3.91094E-02	5.08253E-02	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
4	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

XSEC ID GRP.	63	64	65	66	91	1007	1000	1001
1	9.66101E-04	6.56898E-04	5.15714E-04	3.31133E-04	6.70510E-01	0.00000E+00	4.42718E+00	4.42519E+00
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.04442E+01	1.04449E+01
3	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.08423E+00	6.18360E+01	6.18430E+01
4	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.48424E+01	2.77661E+02	2.77661E+02

93% UO2F2 SOLUTION SPHERE
URANIUM-238 ENDF/B-IV MAT 1262 UPDATED 10/12/89
ZONE WEIGHTED CROSS SECTIONS FOR XSDRN MATERIAL 192238

XSEC ID GRP.	1	2	4	16	18 (σ_f)	17 ($\sigma_{n,3n}$)	27	101
1	7.35008E+00	4.42041E+00	2.43113E+00	3.05715E-02	4.14449E-01	1.97582E-04	4.67767E-01	5.33174E-02
2	1.26278E+01	1.12385E+01	8.18482E-01	0.00000E+00	6.35542E-04	0.00000E+00	5.70847E-01	5.70212E-01
3	7.54774E+01	3.28201E+01	0.00000E+00	0.00000E+00	2.32654E-08	0.00000E+00	4.26572E+01	4.26572E+01
4	1.06356E+01	8.92114E+00	0.00000E+00	0.00000E+00	4.80696E-09	0.00000E+00	1.71446E+00	1.71446E+00

XSEC ID GRP.	102	251 (μ_L)	252 (ξ)	253 (γ)	452 ($\overline{\nu}$)	1099	1018 (χ)	1000
1	5.33174E-02	6.30831E-01	3.12949E-03	4.34977E-03	2.83089E+00	2.80495E-04	7.22663E-01	4.52073E+00
2	5.70212E-01	1.67588E-01	7.05333E-03	5.27418E-03	2.42844E+00	3.50111E-04	2.77344E-01	1.03270E+01
3	4.26572E+01	2.82523E-03	8.45047E-03	5.64161E-03	2.31950E+00	1.41347E-04	6.14482E-06	7.53407E+01
4	1.71446E+00	2.82524E-03	8.45053E-03	5.64164E-03	2.31950E+00	2.05029E-04	1.12230E-09	1.01047E+01

XSEC ID GRP.	1001
1	4.51706E+00
2	1.03303E+01
3	7.53460E+01
4	1.01047E+01

93% UO2F2 SOLUTION SPHERE

CELL AVERAGED FLUXES

ZONE	GRP. 1	GRP. 2	GRP. 3	GRP. 4
1	2.80495E-04	3.50111E-04	1.41347E-04	2.05029E-04
2	2.80495E-04	3.50111E-04	1.41347E-04	2.05029E-04

per unit volume

FLUX DISADVANTAGE FACTORS (ZONE AVERAGE/CELL AVERAGE-FLUX)

ZONE	GRP. 1	GRP. 2	GRP. 3	GRP. 4
1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
2	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

ratios of flux per unit volume in a zone to flux per unit volume in the cell

CELL AVERAGED CURRENTS

ZONE	GRP. 1	GRP. 2	GRP. 3	GRP. 4
1	7.17948E-05	5.58555E-05	1.52069E-05	1.00724E-05
2	7.17948E-05	5.58555E-05	1.52069E-05	1.00724E-05

ZONE	VOLUME	VOL. FRACTION
1	1.71572E+04	1.00000E+00
2	1.71572E+04	1.00000E+00

ELAPSED TIME 0.49 MIN.

18 array 16$ 93% UO2F2 SOLUTION SPHERE
A CCCC ISOTXS INTERFACE WILL BE WRITTEN ON LOGICAL 20

HISONM	HABSID	HMAT
H-1	1001	1269
O-16	8016	1276
F-19	9019	1277
U-235	92235	1261
U-238	92238	1262

ELAPSED TIME 0.49 MIN.

F3.8 OUTPUT CROSS SECTIONS

One of the most common uses of XSDRNPM is to collapse cross sections and write them onto a file for input into another computer code. At present, three options are allowed:

1. Output library in AMPX Working Library format (see Sect. F8.1.1). This library is always written when cross sections are collapsed.

2. Output library in ANISN binary or BCD *format*.[3] The binary library is written on logical 20 by default; the BCD library is produced on logical 7. The identifiers on this library range from 1 to the total number of blocks required to accommodate the data.

3. Output library in the *CCCC*[6] ISOTXS format on logical 20 by default. The set identifiers are! specified in the 18U or 18# array in a one-to-one correspondence with the 16$ array where the identifiers on the XSDRNPM produced working library are specified.

F3.9 ERROR MESSAGES

During the course of a problem, XSDRNPM makes many checks to determine if input data are in the required form. If inconsistencies are spotted, a message is printed, and the problem may be terminated. Some of these messages are listed below along with a brief description of their possible cause.

CORE	N	Insufficient core storage, N = required storage locations.
DATA	N	N arrays have been input with incorrect length. See the messages produced as arrays are read to determine specific arrays.
SN-1	N	The Nth entry in the S_n quadrature directions is zero. (43* array)
SN-2	0	The S_n weights do not sum to 1.0. (42* array)
SN-3	0	The sum of the products of S_n weights and directions is not 0.0, that is, the directions are not symmetric. (42* and 43* arrays)
FIXS	0	Fixed source calculation requested (IEVT=O) and total fixed sources are zero.
Q-HI	N	A volumetric source spectrum numbered N has been requested where N is greater than IQM.
B-HI	N	A boundary source spectrum numbered N has been requested where N is greater than IPM.
FISS	0	IEVT ≥ 1 and the total fission source is zero.
8101	N	The N*th* radius is negative.
8102	N	The N*th* radius is less than the (N-1)*th* radius.
8103	N	Zone N dimensions have become negative in a zone width search.
MIX	N	A request has been made to use the N*th* component from the mixing table, but this nuclide has not been requested from a library.

Several messages may be encountered during an XSDRNPM run which indicate problems with either the code or the setup:

```
********************************************** BT **********************************************
INSUFFICIENT STORAGE FOR BALANCE TABLES
nn WORDS NEEDED, ONLY mm WORDS AVAILABLE
********************************************** DOQ **********************************************
NOT ENOUGH DATA STORAGE AVAILABLE TO GENERATE QUADRATURE DIRECTIONS AND WEIGHTS
nn LOCATIONS NEEDED, BUT ONLY mm LOCATIONS AVAILABLE
********************************************** FEWG **********************************************
INSUFFICIENT STORAGE FOR WEIGHTING— REQUESTED nn LOCATIONS AND HAVE ONLY mm
********************************************** INFACE **********************************************
*** WARNING   YOU REQUESTED nn SETS OF CROSS SECTIONS, BUT ONLY mm SETS WERE FOUND ***
********************************************** MIXEM **********************************************
MAGIC WORD ERROR DETECTED IN MIXEM, MW= xx
********************************************** OUTPUT **********************************************
***** NEED nn WORDS IN OUTPUT, BUT ONLY HAVE mm WORDS *****
********************************************** SPOUT **********************************************
INTERFACE LIBRARY PREPARATION REQUIRED nn LOCATIONS.   PROGRAM ALLOWS mm
********************************************** SPOUT **********************************************
ANISN LIBRARY PREPARATION REQUIRES nn LOCATIONS.    PROGRAM ALLOWS mm
********************************************** SPOUT **********************************************
NO PROGRAMMING PROVIDED FOR ITP= nn
********************************************** FIDAS **********************************************
****** ERROR nn ENTRIES REQUIRED IN xx? ARRAY
 DATA EDIT CONTINUES
********************************************** FIDAS **********************************************
****** FILL OPTION IGNORED IN xx? ARRAY
********************************************** FIDAS **********************************************
****** WARNING ADDRESS aa IS BEYOND LIMITS OF xx? ARRAY
****************************************** XSDRN, O0O001 ******************************************
INSUFFICIENT STORAGE IN XSDRN$
********************************************** STORXS **********************************************
MAGIC WORD ERROR IN STORXS - GROUP gg    MIXTURE mm   L  ln
MAGIC WORD mw    IGI  ig   MXI mx   MNI mn    LLL  ll
********************************************** STORXS **********************************************
ERROR #1 IN STORXS.$
********************************************** STORXS **********************************************
ERROR #2 IN STORXS.$
```

For the cryptic messages above (e.g., the last two), contact the code developers as to their possible cause.

F3.10 REFERENCES

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F3.A SPECIAL XSDRNPM FILES

Two special files that can be optionally produced by XSDRNPM are described in this appendix. (See Sect. F3.5 and the discussion of parameters in the 2$ array.)

F3.A.1 ACTIVITY FILE

The following is the record structure of the activity file which can be produced on logical unit IBLN.

Record 1 - (Title (I),I=1,18),IGM,NNEUT,NGAMM,IM,IAZ,IAI

1. Title - 18 words of text that describe the case. This is the title card from the calculation.
2. IGM - Total number of energy groups.
3. NNEUT - Number of neutron energy groups.
4. NGAMM - Number of gamma energy groups.
5. IM - Number of spatial intervals in the problem.
6. IAZ - Number of "activities" requested to be calculated.
7. IAI - Trigger on whether activities by interval will be determined.

Record 2 - (EN(I),I=1,NNEUT+1)
When NNEUT>0, this record contains the energy boundaries for the neutron group structure (high-to-low).

Record 3 - (EG(I),I=1,NGAMM+1)
When NGAMM>0, this record contains the energy boundaries for the gamma group structure (high-to-low).

Record 4 - (R(I),I=1,IP)
Radii corresponding to all interval boundaries in the system starting at the left side of the system.

Record 5 - (MA(I),I=1,IM)
Zone numbers by interval.

Record 6 - (J3(I),I=1,IAZ)
"Material" numbers for activities.
(This is the 49$ array.)

Record 7 - (J4(I),I=1,IAZ)
"Process" identifiers for activities. (This is the 50$ array.)

These seven records are followed by IAZ records which have the following structure and contain the activities as a function of interval:

(ACT(I),I=1,IM)

F3.A.2 BALANCE TABLE FILE

The structure of the "balance table file" to be written on logical NBL when NBL > 0 is:

Record 1 - AKEFF, SP, IZP, IGP, IBP
1. AKEFF - *keff* for problem
2. SP - search parameter for case
3. IZP - number of zones plus one
4. IGP - number of groups plus one
5. IBP - number of broad groups plus one

Record 2 - (JZM(I),I=1,IM)
Zone numbers by interval for each of IM spatial intervals in the problem.

Record 3 - (V(I),I=1,IM)
Volumes by interval.

Record 4 - (A(I),I=1,IP)
Areas for each boundary of the intervals in the problem, starting at the left-hand boundary.

Record 5 - (WTCOS(M),M=1,MM)
Weights times angle cosines for each angle in the discrete ordinates quadrature.

Record 6 - (WT(M),M=1,MM)
Weights for the directions in the discrete ordinates quadrature.

Record 7 - ((FIX(I,J),I=1,IGP),J=1,IZP)
Fixed sources as a function of energy group I and zone J. Note that the IGP and IZP indexes are for sums over all groups and all zones, respectively.

Record 8 - ((FISS(I,J),I=1,IGP),J=1,IZP)
Fission sources as a function of energy group I and zone J.

Record 9 - ((ABS(I,J),I=1,IGP,J=1,IZP)
Absorptions as a function of group and zone.

Record 10 - ((LEAK(I,J),I=1,IGP),J=1,IZP)
Leakages by group and zone.

Record 11 - ((FRATE(I,J),I=1,IGP),J=1,IZP)
Fission rates as a function of group and zone.

Record 12 - ((FLUX(I,J),I=1,IGP),J=1,IZP)
Volume-integrated fluxes by group and zone.

Record 13 - ((AN2(I,J),I=1,IGP),J=1,IZP)
n2n reaction rates as a function of group and zone.

Record 14 - ((DB2PHI(I,J),I=1,IGP),J=1,IZP)
$DB^2\psi$ transverse leakages by group and zone.

Record 15 - ((CR(I,J),I=1,IGP),J=1,IZP)
Leakage out of the right boundary of the zone by group and zone.

Record 16 - ((CL(I,J),I=1,IGP),J=1,IZP)
Leakage out of the left boundary of the zone by group and zone.

Record 17 - ((ACR(I,J),I=1,IGP),J=1,IZP)
Net currents on the right-hand zone boundaries by group and zone.

Record 18 - ((ACL(I,J),I=1,IGP),J=1,IZP)
Net currents on the left-hand zone boundaries as a function of group and zone.

If IBP > 0

Records 19-30 - Same as Records 7-18 in broad-group structure.

F3.B XSDRNPM PROCESS IDENTIFIERS

Within XSDRNPM, as in most of the rest of SCALE, ENDF/B "MT" numbers are used to identify processes on various input and output arrays. The following table is a copy of information taken from Ref. 18.

Additional identifiers which are either produced or may be encountered are shown at the end of the table.

MT	Description
1	Total cross section (redundant, equal to the sum of all partial cross sections)
2	Elastic scattering cross section
3	Nonelastic cross section (redundant, equal to the sum of all partial cross sections except elastic scattering)
4	Total inelastic cross section (redundant, equal to sum of MT = 51, 52, 53,..., 90, 91)
5	(To be assigned)
6	(n,2n) cross section for first excited state (describes first neutron)
7	(n,2n) cross section for second excited state (describes first neutron)
8	(n,2n) cross section for third excited state (describes first neutron)
9	(n,2n) cross section for fourth excited state (describes first neutron)
10-15	(To be assigned)
16	Direct (n,2n) cross section [total (n,2n) cross section is sum of MT 6, 7, 8, 9, and 16]
17	(n,3n) cross section
18	Total fission cross section (sum of MT = 19, 20, 21, 38).
19	(n,f) cross section (first chance fission)
20	(n,n'f) cross section (second chance fission)
21	(n,2n'f) cross section (third chance fission)
22	(n,n'α) cross section
23	(n,2nα) cross section
24	(n,2nα) cross section
25	(n,3nα) cross section
26	(n,2n) isomeric state cross section
27	Absorption cross section (sum of MT = 18 and 101) includes particle reactions
28	(n,n'p) cross section
29	(n,n'2α) cross section
30	(n,2n2α) cross section

MT	Description
31	Used only in ENDF/B data as an LR flag to indicate that γ-emission is the mode of decay of the residual nucleus formed in the primary reaction[a]
32	(n,n'd) cross section
33	(n,n't) cross section
34	(n,n'^{3}He)
35	(n,n'd2α) cross section
36	(n,n't2α) cross section
37	(n,4n) cross section
38	(n,3nf) cross section (fourth chance fission)
39	Used only in ENDF/B data to indicate that internal conversion is the mode of decay of the residual nucleus formed in the primary reaction[a]
40	Used only in ENDF/B data to indicate that electron-positron pair formation is the mode of decay of the residual nucleus formed in the primary reaction[a]
41-45	(To be assigned)
46	Cross section for describing the second neutron from (n,2n) reaction for first excited state
47	Cross section for describing the second neutron from (n,2n) reaction for second excited state
48	Cross section for describing the second neutron from (n,2n) reaction for third excited state
49	Cross section for describing the second neutron from (n,2n) reaction for fourth excited state (Note: MT = 46, 47, 48, and 49 should not be included in the sum for the total (n,2n) cross section.)
50	(To be assigned)
51	(n,n' to the first excited state
52	(n,n') to the second excited state
.	
.	
.	
90	(n,n') to the 40th excited state
91	(n,n') to the continuum
92-100	(To be assigned)

[a]The "primary" reaction could be, for example, an (n,n'), (n,p), (n,α), (n,n'p), etc., reaction.

MT	Description
101	Neutron disappearance (sum of all cross sections in which a neutron is not in the exit channel), i.e., $$MT = 101 \text{ is } \sum_{i=2}^{14} (MT = 100 + i)$$
102	(n,γ) radiative capture cross section.
103	(n,p) cross section
104	(n,d) cross section
105	(n,t) cross section
106	(n,^{3}He) cross section
107	(n,α) cross section
108	(n,2α) cross section
109	(n,3α) cross section
110	(To be assigned)
111	(n,2p) cross section
112	(n,pα) cross section
113	(n,t2α) cross section
114	(n,d2α) cross section
115-119	(To be assigned)
120	Target destruction = nonelastic less total (n,n′γ)
121-150	(To be assigned)
151	General designation for resonance information
152-200	(To be assigned for specific resonance information)
201-202	(To be assigned)
203	Total hydrogen production
204	Total deuterium production
205	Total tritium production
206	Total ^{3}He production
207	Total ^{4}He production
208-250	(To be assigned)
251	$\overline{\mu}_L$; the average cosine of the scattering angle (laboratory system) for elastic scattering
252	ξ, the average logarithmic energy decrement for elastic scattering

MT	Description
253	γ, the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic decrement for elastic scattering
254-300	(To be assigned)
301-450	Energy release rate parameters, $\overline{E*\sigma}$, for total and partial cross sections. Subtract 300 from this number to obtain the specific reaction type identification, for example, MT = 302 = (300+2) denotes elastic scattering
451	Heading or title information (given only in File 1)
452	$\bar{\nu}$, average total (prompt plus delayed) number of neutrons released per fission event
453	Radioactive nuclide production
454	Fission product yield data
455	Delayed neutrons from fission
456	Prompt neutrons from fission
457	Radioactive decay data
458	Energy release in fission
459-500	(To be assigned)
501	Total photon interaction cross section
502	Photon coherent scattering
503	(To be assigned)
504	Photon incoherent scattering
505-514	(To be assigned)
515	Pair production, electron field
516	Pair production, nuclear and electron field (i.e., pair plus triplet production)
517	Pair production, nuclear field
518	Photofission (γ,f)
519-526	(To be assigned)
527	Sum of all gamma-ray absorption processes
528-531	(To be assigned)
532	Photoneutron (γ,n)
533	Total photonuclear
534-601	(To be assigned)
602	Photoelectric
603-699	(To be assigned)

MT	Description
700	(n,p_0) cross section (cross section for leaving the residual nucleus in the ground state)
701	(n,p_1) cross section for 1st excited state
702	(n,p_2) cross section for 2nd excited state
703	(n,p_3) cross section for 3rd excited state
704	(n,p_4) cross section for 4th excited state
.	
.	
.	
718	(n,p_c) cross section for continuum excited state
719	(n,p_c') cross section for continuum specifically not included in a total (redundant, used for describing outgoing proton)
720	(n,d_0) cross section for ground state
721	(n,d_1) cross section for 1st excited state
722	(n,d_2) cross section for 2nd excited state
.	
.	
.	
738	(n,d_c) cross section for continuum excited state
739	(n,d_c') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing deuteron)
740	(n,t_0) cross section for ground state
741	(n,t_1) cross section for 1st excited state
742	(n,t_2) cross section for 2nd excited state
.	
.	
.	
750	(n,t_c) cross section for continuum excited state
759	(n,t_c') cross section for continuum specifically not included in a σ total (redundant, used for describing outgoing triton)
760	$(n,^3He_0)$ cross section for ground state
761	$(n,^3He_1)$ cross section for 1st excited state
.	
.	
.	
778	$(n,^3He_c)$ cross section for continuum
779	$(n,^3He_c)$ cross section for continuum specifically not included in σ total (redundant, used for describing outgoing ^3He)
780	(n,α_0) cross section for ground state

MT	Description
781	(n,α_1) cross section for 1st excited state
.	
.	
.	
798	(n,α_c) cross section for continuum
799	(n,α_c') cross section for continuum specifically not included in σ_T (redundant, used to describe outgoing α)
800-999	(To be assigned)

The following processes are not "ENDF/B" processes but may be added by various preprocessing codes in the SCALE and/or AMPX systems.

1000	Transport cross section based on the outscatter approximation. See Section F3.2.30
1001	Transport cross section based on the inscatter approximation. See Section F3.2.30
1007	Thermal scattering matrix
1008	Elastic part of thermal scattering matrix
1018	Fission spectrum
1021	These data, which are generated by a preprocessing code for resonance nuclides, are the "bodies" of the $\ell = 0$ resonances for the (n,γ) reaction, weighted over some specified weighting option which is usually 1/E in the resonance region. (The "body" of a resonance is the energy range over which the Nordheim integral treatment is used in the NITAWL-II module to calculate resonance self-shielded data.) When a resonance calculation is not specified for a resonance nuclide in NITAWL-II, the MT = 1021 and MT = 102 data on the master library are summed and identified as the (n,γ) cross section-MT 102 data- in any cross-section library produced by NITAWL-II. (Note that when a 1/E weighting function is used in the resonance range in XLACS-2, the sum of the MT = 1021 and MT = 102 data are, by definition, the infinite dilution cross sections.) When a resonance calculation is triggered in NITAWL-II, the MT = 1021 data are not used.
1022	Fission "body" of the $\ell = 0$ resonance data which is analogous to the MT = 1021 data
1023	Elastic scattering "body" of the $\ell = 0$ resonance data which is analogous to the MT = 1021 data
1099	Group integral of the weight function
1452	Product of υ times the fission cross section
1500-1501	Same as 1000, 1001 except for gamma-ray cross sections
1527	Gamma-ray energy absorption coefficient factors

The various sets of dose conversion factors and their corresponding MT numbers can be found in Table F4.4.1.

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XSDOSE: A MODULE FOR CALCULATING FLUXES AND DOSE RATES AT POINTS OUTSIDE A SHIELD

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ABSTRACT

Under contract with the U.S. Nuclear Regulatory Commission, the Computing Applications Division at Oak Ridge National Laboratory has developed the SCALE system for performing standardized computer analyses for licensing evaluation of nuclear systems. The SCALE system includes a number of selected data libraries, as well as various calculational modules for performing criticality, shielding, and heat transfer analyses.

This document describes the XSDOSE code, which is used in conjunction with XSDRNPM to compute the n/γ flux and the resulting dose at various points outside a finite cylinder or sphere. It may also be used to compute the flux and/or dose at various points due to a finite rectangular surface source or a circular disc. The code assumes that the outgoing angular flux distribution on the rectangle, cylinder, sphere, or disc is independent of position and that the surrounding media is a void. Unlike previous codes, the numerical technique employed in XSDOSE is suitable for points on, close to, or far from the source.

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F4.1 INTRODUCTION

F4.1.1 DEFINITION OF THE PROBLEM SOLVED BY XSDOSE

XSDOSE is a code used in conjunction with XSDRNPM to compute the n/γ flux and the resulting dose at various points outside a finite cylinder or sphere. It may also be used to compute the flux and/or dose at various points due to a finite rectangular surface source or a circular disc. The code assumes that the outgoing angular flux distribution on the rectangle, cylinder, sphere, or disc is independent of position and that the surrounding media is a void. Unlike previous codes, the numerical technique employed in XSDOSE is suitable for points on, close to, or far from the source.

XSDOSE is typically used in conjunction with a fixed-source XSDRNPM calculation for an infinite slab, cylinder, or sphere. XSDOSE then reads the angular flux file produced by XSDRNPM and performs the required numerical integration over a finite surface to obtain the actual scalar flux at those points specified by the user. To the extent that the XSDRNPM angular flux distribution on the surface of the body represents the actual angular flux distribution, XSDOSE will yield an exact solution. XSDOSE is used by the SAS1 (see Sect. S1) and SAS2 (see Sect. S2) shielding analysis sequences.

F4.1.2 DISADVANTAGES OF USING XSDRNPM IN THE EXTERNAL VOID BEYOND A FINITE SURFACE

F4.1.2.1 Inability to Properly Account for the Finite Dimensions of the System

Perhaps the most obvious disadvantage of using a one-dimensional (1-D) code such as XSDRNPM to calculate the n/γ flux or dose rate at a point some distance for the finite dimensions of the system is that, inevitably, the XSDRNPM calculation will be somewhat conservative since the flux or dose at the point of interest would be based on an infinite plane source or an infinite cylindrical source. Far from the surface, this effect could be devastating; close to the surface it may not be too serious.

When using a 1-D code such as XSDRNPM to calculate the flux at a point reasonably close to the surface, people often use a DB^2 buckling correction to account for the finite dimensions of the system in the transverse directions (cf. Sect. C1.3.7). With this correction, the transverse leakage in each energy group is calculated as $D_g B_g^2 \phi_g$ and treated as an absorption term in the transport equation. This approach, however, is only partially satisfying and should probably be avoided in shielding calculations since the DB^2 term represents an isotopic correction in each mesh interval. In reality, some angular fluxes would be affected greatly by the finite dimensions of the system while the most "outward-directed" angular fluxes important in shielding calculations would be affected to a much smaller degree.

F4.1.2.2 Penalty that Must be Paid to Accurately Account for Angular Streaming

In curvilinear geometries it is important to adequately represent the angular streaming terms in the transport equation. This representation is particularly important if one wishes to use a discrete-ordinates code such as XSDRNPM to calculate the n/γ flux or corresponding dose at points some distance from a spherical source or an infinite cylindrical source. In practice, that means using a higher-order angular quadrature and a fairly tight spatial mesh, both inside the body and all the way out to the point of interest. Calculation of the additional angular fluxes in each spatial mesh interval will add to the overall computational burden (i.e., CPU time) and increase the amount of storage required to run the problem.

To illustrate why this extra precision is needed in curvilinear geometries, consider the situation depicted in Fig. F4.1.1 wherein a neutron is shown as traveling from the surface of a spherical body towards the detector at point D. As the particle travels from the surface of the cask towards the detector, the angle it makes with respect to the outward-directed normal changes continually. Indeed, the corresponding angular flux distribution [$\psi(r,\mu)$] at point r becomes more and more forward-directed as r increases. To calculate the scalar flux at r_D requires an accurate knowledge of the angular flux at r_D and that, in turn, requires that the code accurately calculate $\psi(r,\mu)$ at all points in between. To show why that requires a higher-order angular quadrature and a fairly tight spatial mesh, one need only consider the transport equation in spherical geometry:

$$\mu \frac{\partial\psi(r,\mu)}{\partial r} + \frac{1}{r}(1 - \mu^2)\frac{\partial\psi(r,\mu)}{\partial\mu} + \sigma(r)\psi(r,\mu) = S(r,\mu) . \qquad \text{(F4.1.1)}$$

In the external void, $S(r,\mu) = \sigma(r) = 0$, and the transport equation may be written as

$$r \frac{\partial\psi(r,\mu)}{\partial r} = \left(\frac{\mu^2 - 1}{\mu}\right)\frac{\partial\psi(r,\mu)}{\partial\mu} . \qquad \text{(F4.1.2)}$$

To solve this partial differential equation, the various discrete-ordinates codes use a finite-difference approximation for the flux in both space and angle. Given a known distribution on the surface of the cask [$\psi(r_s,\mu)$], the accuracy of the finite-difference solution for the angular flux at points beyond the surface will depend on how accurately one wishes to calculate $\frac{\partial\psi}{\partial r}$ and $\frac{\partial\psi}{\partial\mu}$ (i.e., on the number of spatial mesh intervals and the number of angular directions. Low-order solutions will, of course, be less accurate.

Finally, it should be noted that while high- and low-order discrete-ordinates solutions may both give reasonably accurate estimates of the net current across various concentric surfaces enclosing a sphere or infinite cylinder, the calculated scalar fluxes and corresponding dose rates at distant points may disagree considerably. To understand this point it is important to note that the discrete-ordinates equations used in XSDRNPM are formulated such that, in a void,

$$A_{i+1}\sum_{m=1}^{MM}\mu_m w_m \psi_m(r_{i+1}) = A_i \sum_{m=1}^{MM}\mu_m w_m \psi_m(r_i) . \qquad \text{(F4.1.3)}$$

This formulation ensures that the total net flow of particles ($\underset{\sim}{A}\cdot\underset{\sim}{J}$) through any concentric surface is constant. For the purpose of illustration, assume that we have a spherical source, and that the high- and low-order quadratures can both yield a reasonably good estimate of the leakage (L) from the system. At points far-distant from the source, the angular flux is very forward-peaked and all the angular flux components will be zero, except the most forward-directed component [$\psi_{MM}(r_i)$]. At such a point,

$$\psi_m = \begin{cases} \psi_{MM} & m = MM \\ 0 & m < MM \end{cases} \qquad \text{(F4.1.4a)(F4.1.4b)}$$

and the scalar flux is calculated as

$$\phi = \sum_{m=1}^{MM} w_m \psi_m = w_{MM}\psi_{MM} . \qquad \text{(F4.1.5)}$$

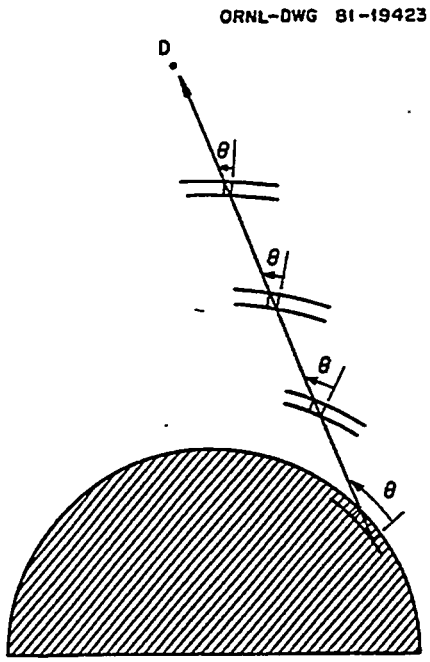


Figure F4.1.1 Changing direction-cosines associated with a free-streaming neutron

Combining Eqs. (F4.1.3), (F4.1.4) and (F4.1.5) yields

$$L = A_s \sum_{m=1}^{MM} \mu_m w_m \psi_m(r_s) = A_i \mu_{MM} w_{MM} \psi_{MM} + A_i \mu_{MM} \phi(r_i) \qquad \text{(F4.1.6)}$$

for $r_i >> r_s$. In other words, the scalar flux calculated by the 1-D discrete-ordinates code will be

$$\phi(r_i) = \frac{(L/A_i)}{\mu_{MM}}, \quad r_i >> r_s . \qquad \text{(F4.1.7)}$$

Given the quadrature sets shown in Table F4.1.1, we see that $\mu_{MM} = 0.86114$ for an S_4 quadrature set and $\mu_{MM} = 0.98940$ for an S_{16} quadrature set. Thus, even though both quadrature sets may correctly calculate the net leakage through the surface at $r = r_i$, the two estimates of the scalar flux [$\phi(r_i)$] may differ by more than 15%.

Table F4.1.1 Various quadrature sets used in spherical geometry

S_2

m	Weights	Directions
1	0	-1.00000E+00
2	5.00000E-01	-5.77350E-01
3	5.00000E-01	5.77350E-01

S_4

m	Weights	Directions
1	0	-1.00000E+00
2	1.73927E-01	-8.61136E-01
3	3.26073E-01	-3.39981E-01
4	3.26073E-01	3.39981E-01
5	1.73927E-01	8.61136E-01

S_8

m	Weights	Directions
1	0	-1.00000E+00
2	5.06143E-02	-9.60290E-01
3	1.11190E-01	-7.96666E-01
4	1.56853E-01	-5.25532E-01
5	1.81342E-01	-1.83435E-01
6	1.81342E-01	1.83435E-01
7	1.56853E-01	5.25532E-01
8	1.11190E-01	7.96666E-01
9	5.06143E-02	9.60290E-01

S_{16}

m	Weights	Directions
1	0	-1.00000E+00
2	1.35762E-02	-9.89401E-01
3	3.11268E-02	-9.44575E-01
4	4.75793E-02	-8.65631E-01
5	6.23145E-02	-7.55404E-01
6	7.47980E-02	-6.17876E-01
7	8.45782E-02	-4.58017E-01
8	9.13017E-02	-2.81604E-01
9	9.47253E-02	-9.50125E-02
10	9.47253E-02	9.50125E-02
11	9.13017E-02	2.81604E-01
12	8.45782E-02	4.58017E-01
13	7.47980E-02	6.17876E-01
14	6.23145E-02	7.55404E-01
15	4.75793E-02	8.65631E-01
16	3.11268E-02	9.44575E-01
17	1.35762E-02	9.89401E-01

F4.1.3 DISADVANTAGES INHERENT IN OTHER PROPOSED METHODS FOR CALCULATING THE SCALAR FLUX AT POINTS BEYOND A FINITE SURFACE

F4.1.3.1 Brief Description of Other Elementary Methods

Given the outgoing angular flux distribution over a finite surface, it is conceptually a rather trivial exercise to calculate the multigroup scalar flux at some distant point. Typically, this is done by integrating the angular flux over the solid angle subtended by the surface as seen from the point of interest, that is

$$\phi = \int_{\Omega \in S} \psi(\underset{\sim}{\Omega}) d\underset{\sim}{\Omega} \ . \tag{F4.1.8}$$

If ρ denotes the radius of a sphere extending from the detector to an arbitrary point on the surface, and $dA_\perp$ denotes the area of a small element on the surface of the sphere, then

$$dA_\perp = \rho^2 d\underset{\sim}{\Omega} = dA_s(\underset{\sim}{a}_n \cdot \underset{\sim}{\Omega}) \ , \tag{F4.1.9}$$

where dA_s represents the area of a small element on the surface of the body (i.e., on the finite rectangular surface source, the finite cylinder, etc.) and $\underset{\sim}{a}_n$ is an outward-directed unit vector normal to the surface of the body. Using Eq. (F4.1.9) to define $d\underset{\sim}{\Omega}$, the equation for the scalar flux may be written as a surface integral over that portion of the body visible from the detector point, that is

$$\phi = \int_S \int \psi(\underset{\sim}{\Omega}) \left(\frac{\underset{\sim}{a}_n \cdot \underset{\sim}{\Omega}}{\rho^2} \right) dA_s \ , \tag{F4.1.10}$$

where $\underset{\sim}{\Omega}$ is a unit vector pointing from the center of the surface element (dA_s) toward the detector point. Given a finite rectangular surface source, as shown in Fig. F4.1.2, and a detector located at (x_D, y_D, z_D), the scalar flux at the point of interest may be written as

$$\phi = \sum_{z_i} \sum_{y_i} \psi(\underset{\sim}{\Omega}_i) \frac{x_D}{[x_D^2 + (y_D - y_i)^2 + (z_D - z_i)^2]^{3/2}} \Delta y_i \, \Delta z_i \ . \tag{F4.1.11}$$

Likewise, if one had a finite cylindrical source, as shown in Fig. F4.1.3, and a detector located at (R_D, Z_D), the scalar flux at the point of interest may be written as

$$\phi = \sum_{z_i} \sum_{\alpha_i} \psi(\underset{\sim}{\Omega}_i) \frac{R_D R_S \cos\alpha_i - R_S^2}{[R_D^2 - 2R_D R_S \cos\alpha_i + R_S^2 + (z_D - z_i)^2]^{3/2}} \Delta\alpha_i \Delta z_i, \tag{F4.1.12}$$

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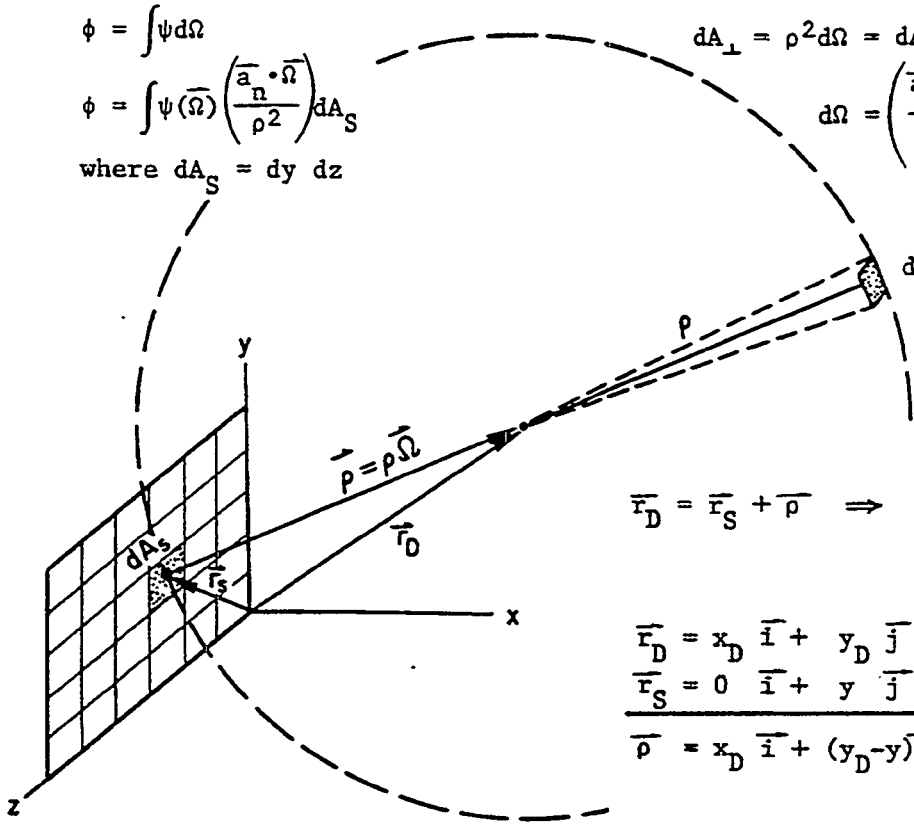
$$\phi = \int \psi d\Omega$$

$$\phi = \int \psi(\vec{\Omega}) \left(\frac{\vec{a}_n \cdot \vec{\Omega}}{\rho^2} \right) dA_S$$

where $dA_S = dy\ dz$

$$dA_\perp = \rho^2 d\Omega = dA_S\ (\vec{a}_n \cdot \vec{\Omega})$$

$$d\Omega = \left(\frac{\vec{a}_n \cdot \vec{\Omega}}{\rho^2} \right) dA_S$$



$$\vec{r}_D = \vec{r}_S + \vec{\rho} \Rightarrow \vec{\rho} = \vec{r}_D - \vec{r}_S$$

$$\vec{r}_D = x_D\,\vec{i} + y_D\,\vec{j} + z_D\vec{k}$$
$$\vec{r}_S = 0\,\vec{i} + y\,\vec{j} + z\,\vec{k}$$
$$\vec{\rho} = x_D\,\vec{i} + (y_D - y)\vec{j} + (z_D - z)\vec{k}$$

$$\rho^2 = x_D^2 + (y_D - y)^2 + (z_D - z)^2$$

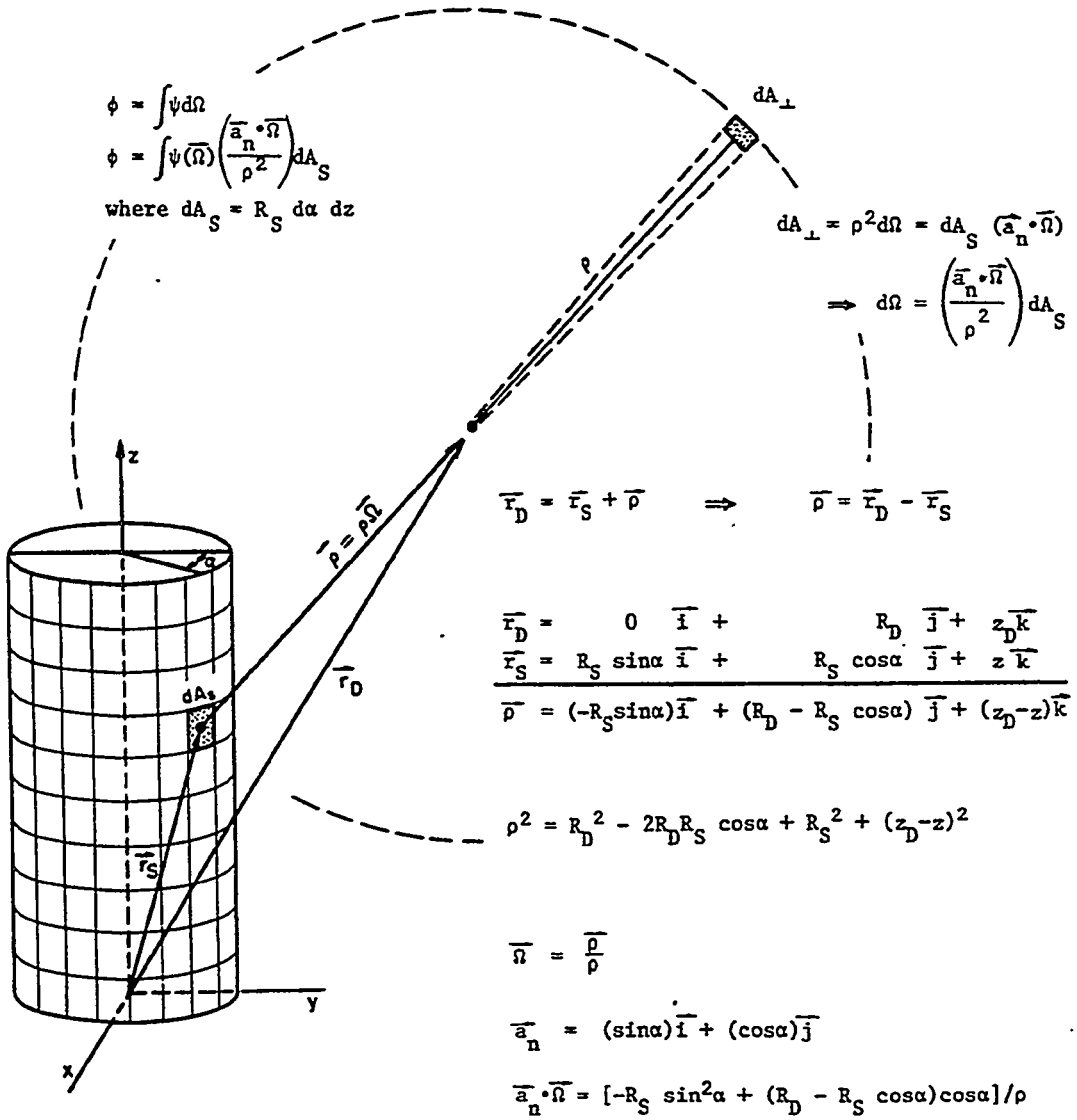
$$\vec{\Omega} = \frac{\vec{\rho}}{\rho} \quad \text{and} \quad \vec{a}_n = \vec{i} + 0\vec{j} + 0\vec{k}$$

$$\vec{a}_n \cdot \vec{\Omega} = \frac{\vec{\rho} \cdot \vec{i}}{\rho} = \frac{x_D}{\rho}$$

$$\phi = \sum_{z_i} \sum_{y_i} \psi(\vec{\Omega}_i) \left[\frac{x_D}{[x_D^2 + (y_D - y_i)^2 + (z_D - z_i)^2]^{3/2}} \right] \Delta y_i\ \Delta z_i$$

Figure F4.1.2 Vector diagram illustrating an elementary procedure for calculating the scalar flux at a point some distance from a rectangular surface source of finite extent

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$$\phi = \sum_{z_i} \sum_{\alpha_i} \psi(\vec{\Omega}_i) \left[\frac{R_D R_S \cos\alpha_i - R_S^2}{[R_D^2 - 2R_D R_S \cos\alpha_i + R_S^2 + (z_D - z_i)^2]^{3/2}} \right] \Delta\alpha_i \, \Delta z_i$$

Figure F4.1.3 Vector diagram illustrating an elementary procedure for calculating the scalar flux at a point some distance from a cylindrical surface source of finite length

where α is the polar angle used to subdivide the cylindrical surface. In either case, the value of the angular flux corresponding to $\underset{\sim}{\Omega}_i$ must be estimated based on a known distribution $\{\psi(\underset{\sim}{r}_s, \underset{\sim}{\Omega}_m); m = 1,2,...,MM\}$ in a few discrete directions $\{\underset{\sim}{\Omega}_m = \mu_m\vec{i} + \eta_m\vec{j} + \xi_m\vec{k}; m = 1,2,...,MM\}$ defined by the particular quadrature set (cf. Fig. F4.1.4). Typically, $\psi(\underset{\sim}{\Omega}_i)$ is defined as $\psi_{m*}(\underset{\sim}{r}_s)$ where $\underset{\sim}{\Omega}_{m*}$ is the quadrature direction closest to $\underset{\sim}{\Omega}_i$. In cylindrical geometry, $\underset{\sim}{\Omega}_m = \mu_m\vec{i} + \eta_m\vec{j} + \xi_m\vec{k}$, and m* is such that $\underset{\sim}{\Omega}_i \cdot \underset{\sim}{\Omega}_{m*} > \underset{\sim}{\Omega}_i \cdot \underset{\sim}{\Omega}_m$ for $m \neq m^*$. In spherical and slab geometry, m* is such that

$$\mu_i\mu_{m*} + \eta_i\sqrt{1-\mu_{m*}^2-\xi_i^2} > \mu_i\mu_m + \eta_i\sqrt{1-\mu_m^2-\xi_i^2},\ m \neq m^*\ , \tag{F4.1.13}$$

or

$$(\arccos(\mu_{m*}) - \arccos(\mu_i))^2 < (\arccos(\mu_m) - \arccos(\mu_i)\}^2\ ,\ m \neq m^*\ . \tag{F4.1.14}$$

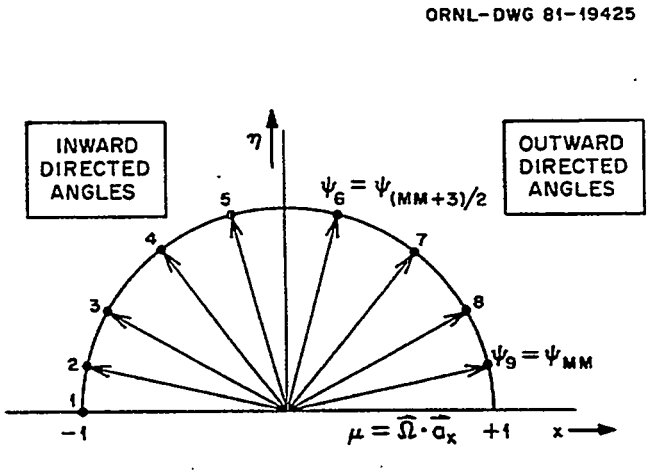


Figure F4.1.4 Ordering of quadrature angles used in slab geometry [Note that for an S_8 quadrature, one has nine angles (MM = ISN + 1)]

F4.1.3.2 Sensitivity of Mesh Size Requirements to the Location of the Detector Relative to the Surface

Even though the method described above is fairly straightforward, it has several disadvantages. The first and most obvious stems from the fact that the integral over $d\underset{\sim}{\Omega}$ has been transformed to a two-dimensional (2-D) surface integral over y and z (or α and z). Immediately this raises the question: How many mesh intervals should be used in the two directions? The answer obviously depends on the size of the surface and how far the detector point is from the surface. If the detector point is relatively far from a rather small surface ($x_D >> y_{surf}^{max}$ and $x_D >> z_{surf}^{max}$), then only a few mesh intervals may be required since all angular flux components reaching the detector point will be forward-directed within a relatively narrow range of solid angle. Closer to the surface, however, this question becomes more important since the number of mesh

intervals determines the accuracy with which we can sample from the angular flux distribution on the surface. To illustrate, consider the rectangular surface source as being divided into a fixed number of mesh intervals in both directions, with the detector located directly in front of mesh interval j such that $(y_D - y_j)^2 + (z_D - z_j)^2 = 0$. Equation (F4.1.1) would then yield

$$\phi = \psi_{MM}\left(\frac{\Delta y_j}{x_D}\right)\left(\frac{\Delta z_j}{x_D}\right) + \sum_{z_i}\sum_{y_i}^{i\neq j} \psi(\underset{\sim}{\Omega}_i)\,\frac{x_D}{[x_D^2+(y_D-y_i)^2+(z_D-z_i)^2]^{3/2}}\Delta y_i \Delta z_i \qquad \text{(F4.1.15a)}$$

$$= \psi_{MM} W + \sum_{i\neq j} \psi_{(MM+3)/2}\, f_i\, \Delta y_i\, \Delta z_i \qquad (\text{as } x_D \to 0)\ , \qquad \text{(F4.1.15b)}$$

where ψ_{MM} denotes the most forward-directed angular flux component associated with the given quadrature set (cf. Fig. F4.1.4), $\psi_{(MM+3)/2}$ denotes the outward-directed angular flux component that is "most tangential" to the rectangular surface, and $f_i \to 0.0$ as $x_D \to 0$. On physical grounds one can argue that the user should select a mesh spacing small enough that W [defined here as $(\Delta y_j\, \Delta z_j)/x_D^2$] is less than 2π. Even that, however, would overweight the forward-directed angular flux component (ψ_{MM}), thereby causing Eq. (F4.1.15) to overestimate the scalar flux in many of the fast energy groups. At the same time, Eq. (F4.1.15) would not properly account for the angular flux in the other various directions as $x_D \to 0$. Use of a still finer mesh spacing would partially remedy this last difficulty, but could lead to an extraordinary number of mesh intervals and increase the overall computing time required. In the end, the user must experiment by trial and error to determine a mesh spacing that is adequate for his/her particular problem.

F4.1.3.3 Inconsistencies Produced by Simplistic Angular Flux Selection Criteria

The second difficulty with the above method stems from the manner in which the values of $\psi(\underset{\sim}{\Omega}_i)$ are determined from the known angular flux distribution $\{\psi(\underset{\sim}{r}_s, \underset{\sim}{\Omega}_m);\ m = 1,2,\ldots,MM\}$. As noted above, $\psi(\underset{\sim}{\Omega}_i)$ in Eq. (F4.1.11) or (F4.1.12) is typically defined as $\psi_{m*}(\underset{\sim}{r}_s)$, where $\underset{\sim}{\Omega}_{m*}$ is the quadrature direction closest to $\underset{\sim}{\Omega}_i$. Using this procedure, it is generally impossible to obtain the exact same result produced by XSDRNPM at points close to the surface, even if one has an infinitely fine spatial mesh (Δy_i, Δz_i)! To illustrate this point, we note that in the limit, as $\Delta y_i \to 0$ and $\Delta z_i \to 0$, Eq. (F4.1.11) is equivalent to Eq. (F4.1.8) which, for an infinite planar source, may be written as

$$\phi = \int_{\Omega\in S} \psi(\underset{\sim}{\Omega})\, d\underset{\sim}{\Omega} = 2\pi\int_0^1 \psi(\mu)d\mu \doteq 2\pi\sum_{i=1}^{N} \psi(\mu_i)\Delta\mu_i\ , \qquad \text{(F4.1.16a)}$$

where $\Delta\mu_i = (1/N) \to 0.0$ as $N \to \infty$,

and $\psi(\mu_i) \equiv \psi(\underset{\sim}{r}_s, \mu_{m*})$, (F4.1.16b)

where m* is such that

$$(\arccos(\mu_{m^*}) - \arccos(\mu_i))^2 < (\arccos(\mu_m) - \arccos(\mu_i))^2,\ m \neq m^* . \qquad \text{(F4.1.16c)}$$

Repeated application of this selection criteria for $\psi(\mu_i)$ would, as $N \to \infty$, yield

$$\phi = \sum_{m=M}^{MM} 2\pi[\cos(\bar{\theta}_{m+1}) - \cos(\bar{\theta}_m)]\psi(\underset{\sim}{r}_s,\mu_m) , \qquad \text{(F4.1.17a)}$$

where $M = (MM + 3)/2$ and (F4.1.17b)

$$\bar{\theta}_m = \begin{cases} = (\pi/2) & , m = (MM + 3)/2 \quad \text{(F4.1.17c)} \\ = (0.5)\,[\arccos(\mu_m) = \arccos(\mu_{m-1})] & , (MM + 5)/2 \le m \le MM \quad \text{(F4.1.17d)} \\ = 0 & , m = MM + 1 \quad \text{(F4.1.17e)} \end{cases}$$

Defining ψ^* in terms of the angular flux per steradian ($\psi^* = 4\pi\psi$), this calculated result as $N \to \infty$ may be written as

$$\phi = \sum_{m=M}^{MM} W_m\, \psi^*(\underset{\sim}{r}_s,\mu_m) , \qquad \text{(F4.1.18a)}$$

where the "effective weights" based on the above selection criteria are given by

$$W_m \equiv (0.5)[\cos(\bar{\theta}_{m+1}) - \cos(\bar{\theta}_m)] . \qquad \text{(F4.1.18b)}$$

By way of comparison, we note that the XSDRNPM result for the scalar flux at the surface may be written as

$$\phi = \sum_{m=M}^{MM} w_m\psi^*(\underset{\sim}{r}_s,\mu_m)\ [\psi^*(\underset{\sim}{r}_s,\mu_m) = 0 \text{ for } m < M] , \qquad \text{(F4.1.19)}$$

where the individual weights $\{w_m\}$ used by XSDRNPM are related to the Gaussian weights of a Legendre polynomial, as shown in Sect. C1.3.6. The point to be made here, of course, is that the "effective weights" $\{W_m\}$ obtained by repeated application of the above selection criteria for $\psi(\mu_i)$ will, as $N \to \infty$, be somewhat different than those used by XSDRNPM. As a result, the two estimates of the scalar flux may be somewhat different even if one uses an infinitely fine mesh in his surface integration! Since the selection criteria is somewhat arbitrary in the first place, XSDOSE uses a different approach which, while still arbitrary, assures some degree of consistency in the limit. Also important in XSDOSE is the fact that the surface integration is performed in such a way that the calculated results are very insensitive to (and essentially independent of) the location of the detector relative to the surface. This unique feature removes the aforementioned uncertainty in determining an adequate mesh size for a particular application.

F4.2 THEORY

F4.2.1 CALCULATION OF THE SCALAR FLUX AT POINTS OUTSIDE A SPHERICAL BODY

To determine the scalar flux at a point some distance from the surface of a spherical source, XSDOSE numerically integrates what appears to be the angular flux at that point:

$$\phi_D = \int \psi(\underset{\sim}{\Omega},r_D)d\underset{\sim}{\Omega} = 2\pi\int_{\cos(\varphi_0)}^{1.0} \psi(\mu_\varphi,r_D)d\mu_\varphi \ , \qquad \text{(F4.2.1a,b)}$$

where $\mu_\varphi = \cos\varphi$, and φ_0 is the maximum angle subtended by the sphere as seen from the detector at $r=r_D$. As shown in Fig. F4.2.1, φ_0 is given by

$$\varphi_0 = \arcsin\left(\frac{r_S}{r_D}\right) , \qquad \text{(F4.2.2)}$$

where r_S is the radius of the spherical source. In practice, Eq. (F4.2.1b) is evaluated numerically by breaking the range of integration [$\cos\varphi_0 < \mu\varphi < 1.0$] into N equal intervals (specified in the input data as NINCRM; typically ~200). Denoting the upper and lower bounds of each interval as $\mu^+_{\varphi_i}$ and $\mu^-_{\varphi_i}$, the characteristic angle for each interval is defined as

$$\varphi_i = 0.5\,[\arccos(\mu^+_{\varphi_i}) + \arccos(\mu^-_{\varphi_i})] . \qquad \text{(F4.2.3)}$$

The integral defined by Eq. (F4.2.1b) is then evaluated as

$$\phi_D = 2\pi \sum_{i=1}^{N} \psi(\mu_{\varphi_i},r_D)\ \Delta\mu_{\varphi_i} = 2\pi\left(\frac{1-\cos\varphi_0}{N}\right)\sum_{i=1}^{N} \psi(\mu_{\varphi_i},r_D) . \qquad \text{(F4.2.4a,b)}$$

From Fig. F4.2.2a, we see that those neutrons that stream past the detector at a fixed angle (φ_i) are the same ones that left the surface of the sphere at an angle γ_i relative to $\underset{\sim}{r}_S$. To determine the angle γ_i corresponding to φ_i, we first apply the Law of Sines to determine the complementary angle α (cf. Fig. F4.2.2b). From Fig. F4.2.2b it is obvious that

$$\frac{\sin\alpha}{r_D} = \frac{\sin\varphi}{r_S} . \qquad \text{(F4.2.5)}$$

Noting that $\alpha > 90°$ whenever $\varphi < 90°$, α must be given by

$$\alpha = \pi - \arcsin\left[\left(\frac{r_D}{r_S}\right)\sin\varphi\right] . \qquad \text{(F4.2.6)}$$

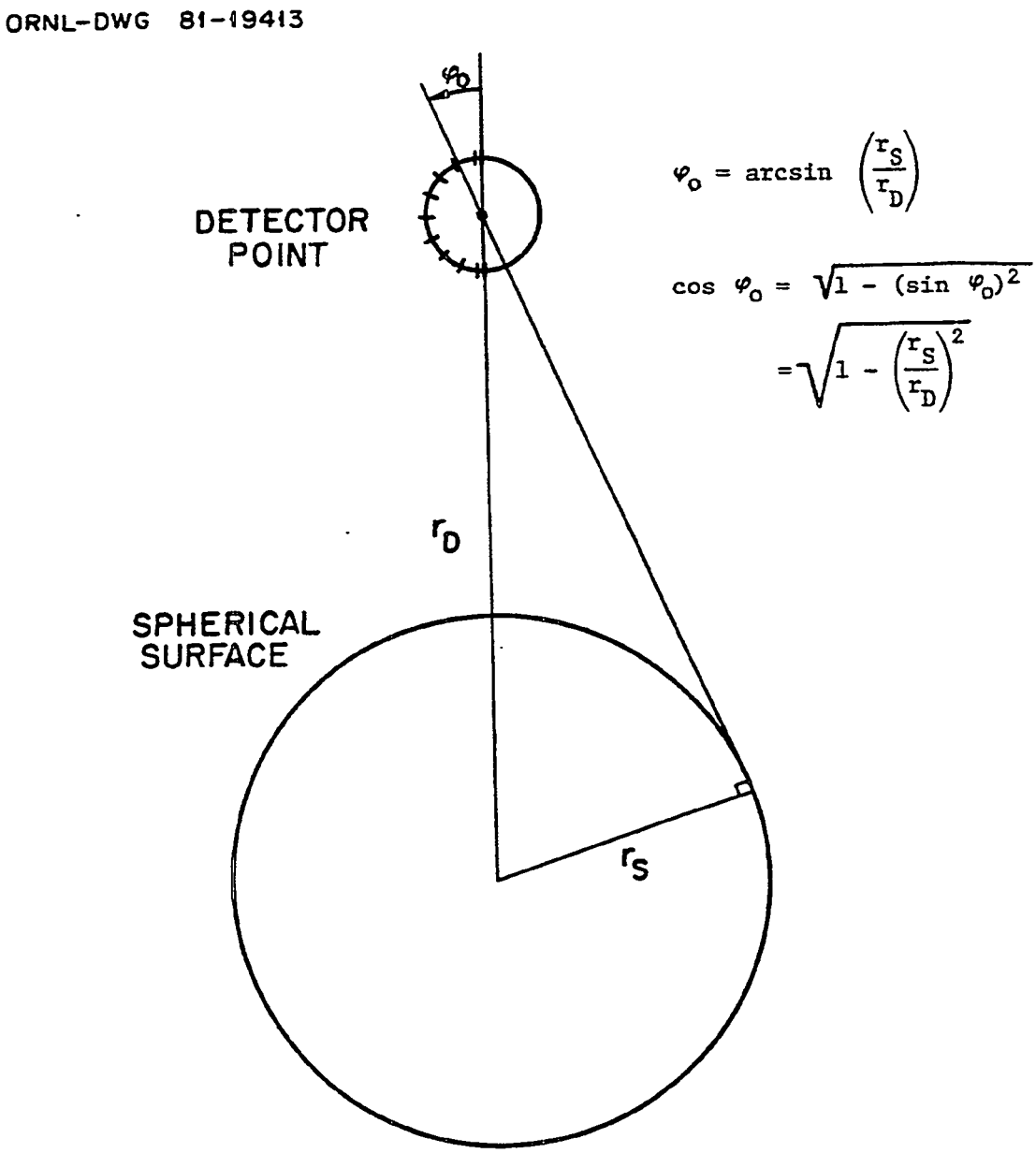


Figure F4.2.1 Sketch showing the maximum angle (φ_0) subtended by a sphere, as seen from a point (D) some distance away

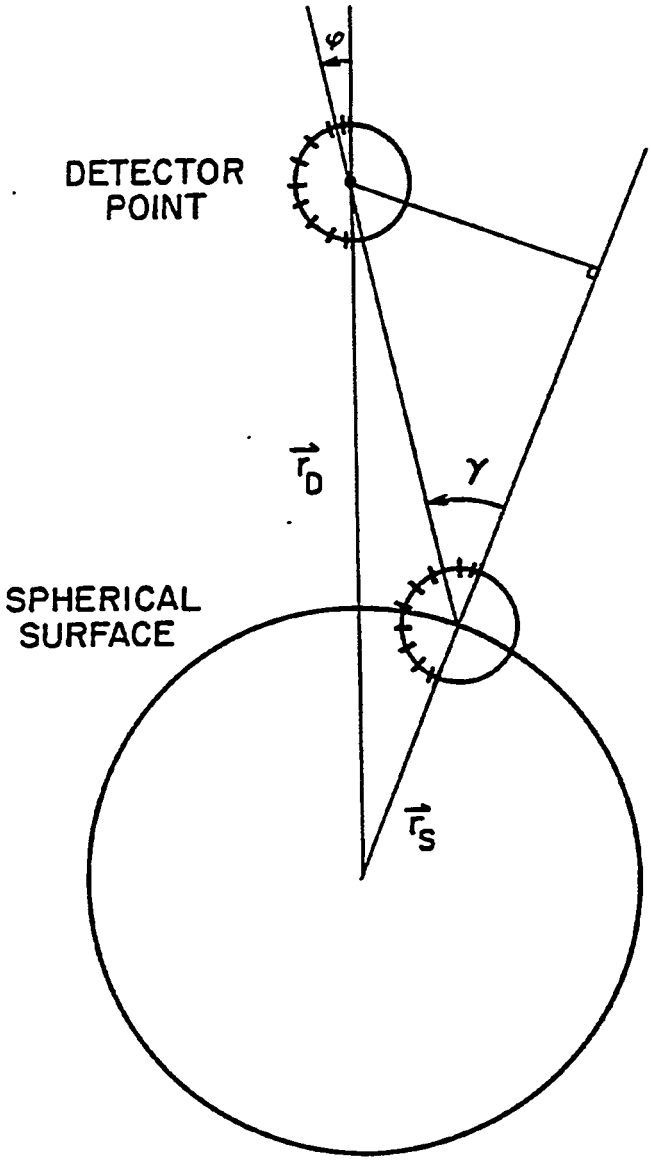
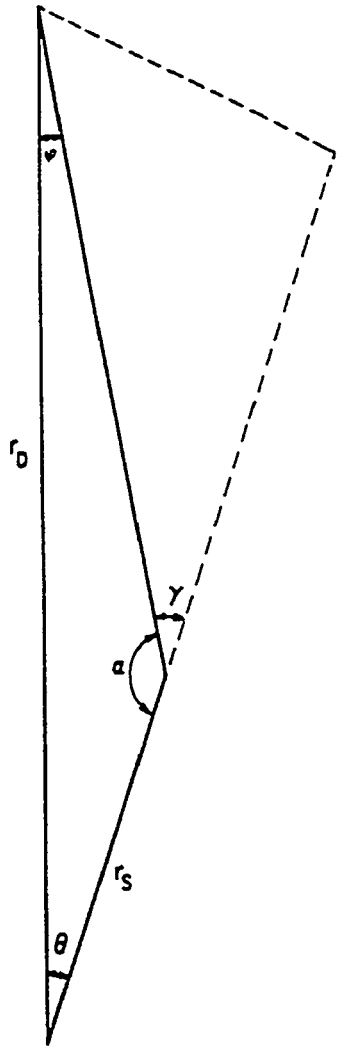


Figure F4.2.2a Sketch showing the physical relationship between the angular flux components at the detector point and the angular flux components on the surface of a sphere

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$$\frac{\sin \alpha}{r_D} = \frac{\sin \varphi}{r_S}$$

$$\alpha = \arcsin \left[\left(\frac{r_D}{r_S} \right) \sin \varphi \right] \qquad \alpha \leq 90°$$

$$\alpha = \pi - \arcsin \left[\left(\frac{r_D}{r_S} \right) \sin \varphi \right] \qquad \alpha \geq 90°$$

$$\alpha + \gamma = \pi$$

$$\gamma = \arcsin \left[\left(\frac{r_D}{r_S} \right) \sin \varphi \right] \qquad \varphi \leq 90°$$

Figure F4.2.2b Sketch showing the mathematical relationship between the angular flux components at the detector point (angle φ) and the angular flux components on the surface of a sphere (angle γ) (See Fig. F4.2.2a for additional details)

Since $\alpha + \gamma = \pi$, γ must be given by

$$\gamma_i = \arcsin\left[\left(\frac{r_D}{r_S}\right) \sin \varphi_i\right], \tag{F4.2.7}$$

and the angular flux $\psi(\mu_{\varphi_i}, r_D)$ is given by

$$\psi(\mu_{\varphi_i}, r_D) = \psi(\mu_{\gamma_i}, r_S) , \tag{F4.2.8a}$$

where

$$\mu_{\gamma_i} = \frac{\underset{\sim}{\Omega} \cdot \underset{\sim}{r}_S}{r_S} = \cos \gamma_i . \tag{F4.2.8b}$$

Knowing μ_{γ_i} and the surface flux in certain discrete directions $\{\psi(\mu_m, r_s), m = 1,...,MM\}$, we need only decide what value to assign $\psi(\mu_{\gamma_i}, r_s)$ at each point (I = 1,...,N). Any procedure used for making this selection would, of course, be somewhat arbitrary. One common procedure is to assign $\psi(\mu_{\gamma_i}, r_s)$ the value of the angular flux (ψ_m) whose direction cosine μ_m is closest to μ_{γ_i}. Unfortunately, if the detector point is sufficiently close to the surface, that procedure will often yield a scalar flux which differs form that calculated by XSDRNPM. To eliminate such differences, XSDOSE uses an alternative procedure that is more consistent with that used in XSDRNPM.

To calculate the scalar flux at any point within the system (or on the surface of the system) XSDRNPM takes a weighted sum of the angular fluxes (ψ_m) in each of the various directions (μ_m) associated with the given quadrature $\{w_m, \mu_m\}$;

$$\phi = \sum_{m=1}^{MM} w_m \psi_m . \tag{F4.2.9}$$

Even though the direction cosines and quadrature weights are predetermined by XSDRNPM in a way that ensures accurate determination of the first N moments of the angular flux,* the weights may (in a simplistic sense) be viewed as the solid angle over which the corresponding angular flux is considered constant[$\psi(\mu) \doteq \psi_m$].** Figure F4.2.3 shows the angular directions corresponding to an S_{10} quadrature in spherical geometry.

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*Given the order of the quadrature (ISN) and the type of geometry (IGE), XSDRNPM and XSDOSE both follow the same procedure for determining the direction cosines $\{\mu_m\}$ and quadrature weights $\{w_m\}$. See Sect. M7.2.5.7 for additional details.

**This simplistic scheme for determining μ_m^- and μ_m^+ is somewhat arbitrary. Note, for example, that one could specify a quadrature set in which μ_m falls outside the range (μ_m^-, μ_m^+). That, however, is very rarely the case. Indeed, the scheme proposed here for determining (μ_m^-, μ_m^+) and subsequently assigning $\psi(\mu_{\gamma_i}, r_s)$ some value [$\psi_m(r_s)$] based on μ_{γ_i} is no more arbitrary than other schemes that have been proposed. In addition, the present scheme allows XSDOSE to faithfully reproduce the scalar fluxes calculated by XSDRNPM whenever the detector point (r_D) is arbitrarily close to the surface (r_S).

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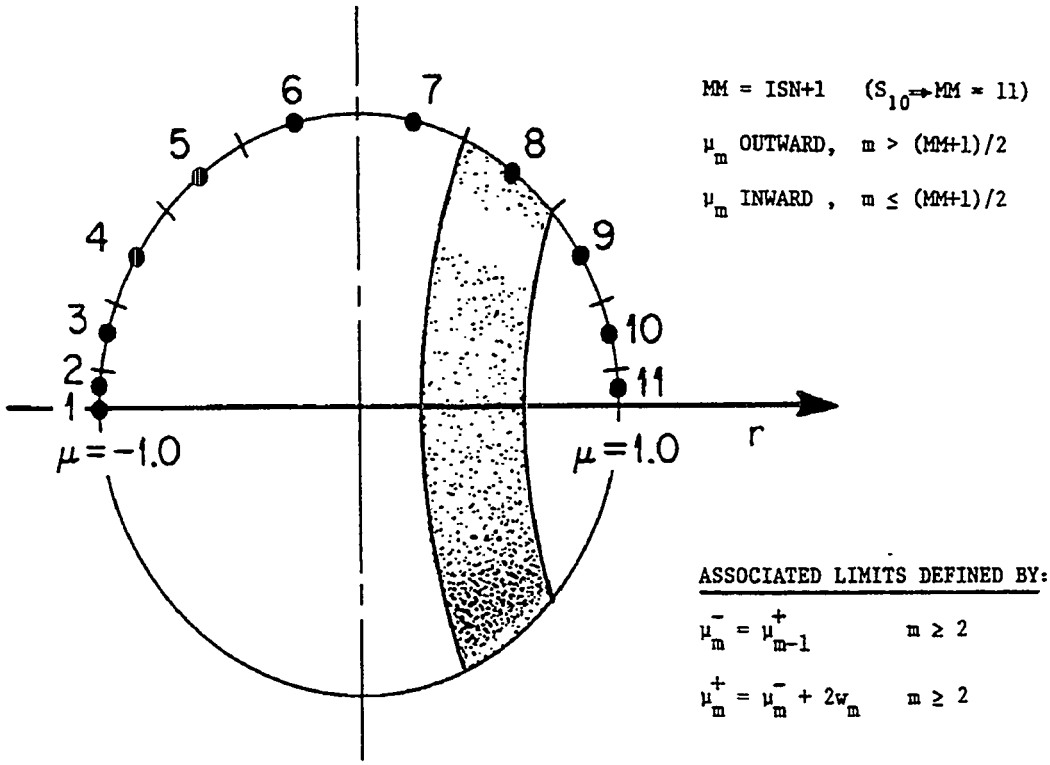


Figure F4.2.3 Solid angle associated with the various direction cosines of discrete-ordinates quadrature sets used in slab and/or spherical geometry (IGE = 1 or IGE = 3)

In addition, it illustrates the limits (μ_m^-, μ_m^+) over which $\psi(\mu) \doteq \psi_m$. Noting that $\mu_1 = -1.0$ and $w_1 = 0.0$, the solid angles (Ω_m) associated with the other discrete directions may be defined in terms of

$$\mu_m^- = \mu_{m-1}^+ , \qquad m \geq 2 \tag{F4.2.10a}$$

and

$$\mu_m^+ = \mu_m^- + 2w_m , \qquad m \geq 2 . \tag{F4.2.10b}$$

Given a specific angular direction (μ_{γ_i}), XSDOSE then assigns $\psi(\mu_{\gamma_i}, r_s)$ the value of the angular flux (ψ_m) whose associated range (μ_m^-, μ_m^+) includes μ_{γ_i}.

It was stated above that Eq. (F4.2.1b) is evaluated numerically by breaking the range of integration ($\cos\varphi_0 < \mu_\varphi < 1.0$) into N equal intervals. While that statement is essentially correct, the actual method was programmed slightly differently for reasons that will become clear below. In practice, $\cos\varphi_0 < \mu_\varphi < 1.0$ is broken into several large "macro" ranges defined by $\cos\varphi_0 < \mu_\varphi < \mu_m^+$ and/or $\mu_m^- < \mu_\varphi < \mu_m^+$. Each of the large "macro" ranges are then subdivided into N_m equal intervals where

$$N_m = 1 + \text{INT}\left\{N\left(\frac{\mu_m^+ - \mu_m^-}{1 - \cos\varphi_0}\right)\right\}, \qquad \cos\varphi_0 < \mu_m^- < \mu_\varphi < \mu_m^+ \qquad \text{(F4.2.11a)}$$

or

$$N_m = 1 + \text{INT}\left\{N\left(\frac{\mu_m^+ - \cos\varphi_0}{1 - \cos\varphi_0}\right)\right\}, \qquad \mu_m^- < \cos\varphi_0 < \mu_\varphi < \mu_m^+ . \qquad \text{(F4.2.11b)}$$

Denoting the upper and lower bounds of each "miniature" interval as $\mu_{\varphi_i}^+$ and $\mu_{\varphi_i}^-$, the numerical determination of ϕ_D proceeds exactly as described above. The only difference is that $\Delta\mu_{\varphi_i}$ used in Eq. (F4.2.4a) may vary slightly from one "macro" range to the next. The advantage of this renormalization within each large "macro" range is that no single interval $\Delta\mu_{\varphi_i}$ "straddles" any of the previously defined angular ranges (μ_m^-, μ_m^+) at the detector site (r_D). As the detector is moved closer and closer to the surface of the sphere (i.e., as $r_D \to r_S$), the code is then able to faithfully reproduce the XSDRNPM surface flux even if $N_m = 1$.]

F4.2.2 CALCULATION OF THE SCALAR FLUX AT POINTS SOME DISTANCE FROM A RECTANGULAR SURFACE SOURCE OR A FLAT CIRCULAR DISC

F4.2.2.1 General Formulation for Calculating the Scalar Flux at Points Some Distance from a Flat Surface Source

Before explaining how XSDOSE calculates the scalar flux at a point some distance from a rectangular surface source or a flat circular disc (representing the end of a cylinder), it is helpful to review how it might calculate the scalar flux at a point some distance (x) away from an infinitely large, flat surface source. In such a situation, $\phi_D(x)$ will obviously be independent of x, and identical to the flux at the surface (ϕ). Nevertheless, understanding the procedure described below will be most helpful in understanding the procedure used in the other two cases of more practical interest.

To determine the scalar flux at a point some distance from a flat surface, XSDOSE numerically integrates what appears to be the angular flux at that point:

$$\phi_D = \int \psi(\underset{\sim}{\Omega}, \underset{\sim}{r}_D) d\underset{\sim}{\Omega} = \iint \psi(\theta, \mu_\varphi, \underset{\sim}{r}_D) d\mu_\varphi d\theta , \qquad \text{(F4.2.12)}$$

where $\mu_\varphi = \cos\varphi = \underset{\sim}{\Omega}\cdot\underset{\sim}{a}_x$. Because the surface is flat, the angle φ shown in Fig. F4.2.4b is the same as γ, and $\mu_\varphi = \mu_\gamma = \underset{\sim}{\Omega}\cdot\underset{\sim}{a}_n$ where $\underset{\sim}{a}_n$ is the outward-directed unit vector normal to the surface. The angle θ used in Eq. (F4.2.12) is, of course, the azimuthal angle shown in Fig. F4.2.4a. In the special case where the

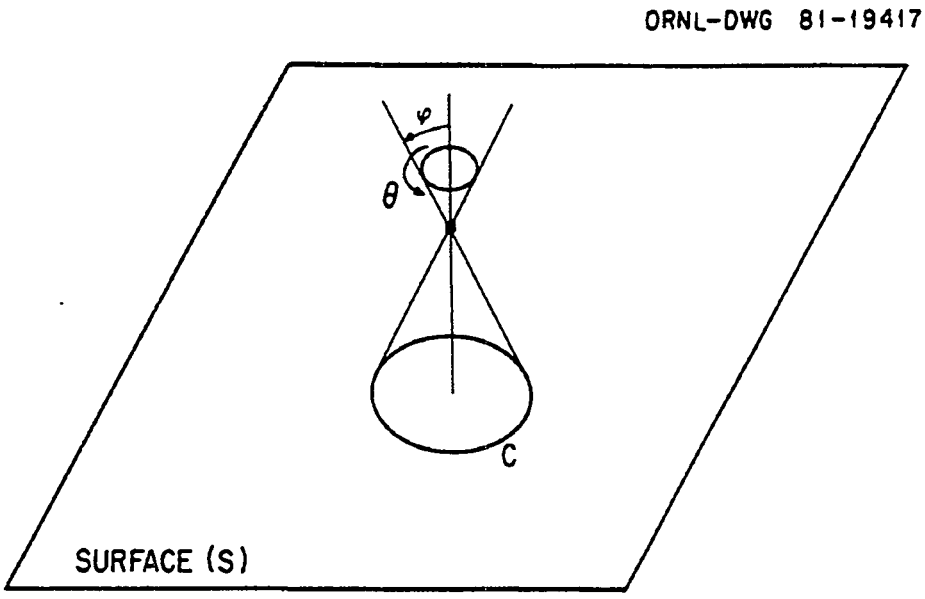


Figure F4.2.4a Flat surface containing a circular line (C) corresponding to the integration of the angular flux (at the detector site) in the azimuthal direction (θ)

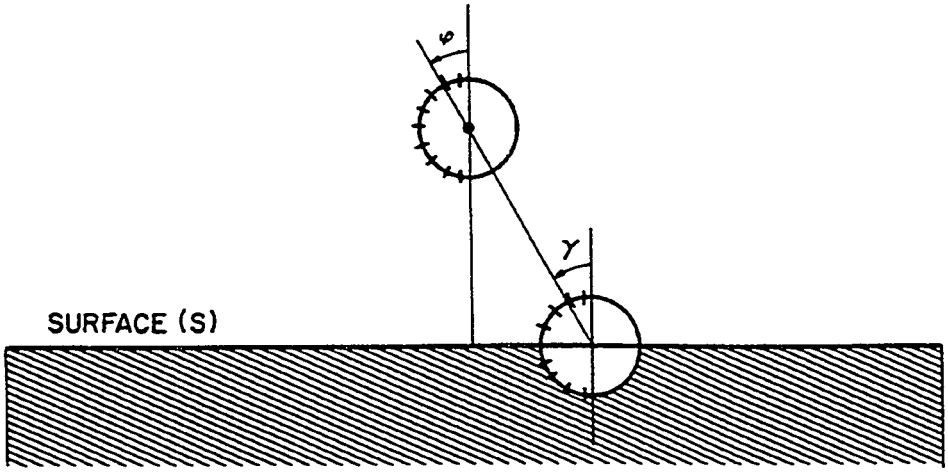


Figure F4.2.4b Sketch showing the relationship between the angular flux components at the detector point (angle φ) and the angular flux components emanating from a flat surface (angle γ). Because the surface is flat, $\varphi = \gamma$

detector (x_D, y_D, z_D) is located directly over some point on the finite surface (y_D, z_D, $\in$ S), Eq. (F4.2.12) may be written as

$$\phi_D = 2\pi \int_{\cos(\varphi_0^-)}^{1.0} f_{C\varphi} \psi_S(\mu_\gamma) d\mu_\gamma \,, \qquad \text{(F4.2.13)}$$

where

$\varphi_0^- = \gamma_0^-$ is the maximum angle subtended by the finite surface (S) as seen from the detector at x_D, y_D, z_D (cf. Fig. F4.2.5b), and

$f_{C\varphi} = f_{C\gamma}$ is the fraction of the circular line (C), corresponding to angle $\varphi(\varphi = \gamma)$, which lies on the finite surface (S); obviously if the surface (S) is infinite in all directions, then $f_{C\gamma} = 1.0$ ($0 < \varphi < 90°$); for finite surfaces, $f_{C\gamma}$ must be determined as explained in Sect. F4.2.2.2 or Sect. F4.2.2.3.

In the more general case where the detector point $\underset{\sim}{r}_D$ is offset with respect to the finite surface (y_D, $z_D \notin$ S), Eq. (F4.2.12) may be written as

$$\phi_D = 2\pi \int_{\cos(\varphi_0^-)}^{\cos(\varphi_0^+)} f_{C\varphi} \psi_S(\mu_\gamma) d\mu_\gamma \,, \qquad \text{(F4.2.14)}$$

where

$\varphi_0^+ = \gamma_0^+$ is the minimum angle subtended by the finite surface (S) as seen from the detector at x_D, y_D, z_D (cf. Fig. F4.2.5b).

The equations used to determine $\cos(\varphi_0^-)$, $\cos(\varphi_0^+)$, and $f_{C\varphi}$ will, of course, depend on whether one has a rectangular surface source or a flat circular disc (representing the end of a cylinder). In either case Eq. (F4.2.14) may be evaluated numerically by breaking the range of integration $\cos(\varphi_0^-) < \mu_\gamma < \cos(\varphi_0^+)$ into N equal intervals (specified in the input data as NINCRM; typically ~200).* Denoting the upper and lower bounds of each interval as $\mu_{\gamma_i}^+$ and $\mu_{\gamma_i}^-$, the characteristic angle for each interval is defined as

$$\gamma_i = \arccos(\mu_{\gamma_i}) \,, \qquad \text{(F4.2.15a)}$$

where

$$\mu_{\gamma_i} = 0.5[(\mu_{\gamma_i}^+) + (\mu_{\gamma_i}^-)] \,. \qquad \text{(F4.2.15b)}$$

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*In practice, the range of integration is really divided into several large "macro" ranges, as described in the concluding paragraph of Sect. F4.2.1. These ranges are then subdivided into many small sub-intervals, as given by Eqs. (F4.2.11a) and (F4.2.11b). The total number of sub-intervals used in the numerical integration will still be ~N. Proceeding in this fashion allows XSDOSE to faithfully reproduce the XSDRNPM results at the surface, even if N is quite small.

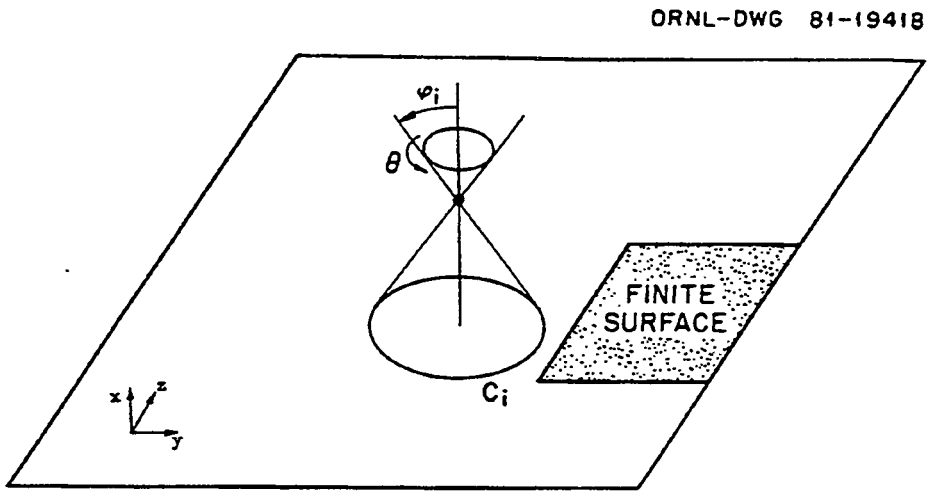


Figure F4.2.5a Flat finite surface lying just to the right of a particular circular line (C_i) corresponding to the integration of the angular flux (at the detector site) in the azimuthal direction (θ) while $\varphi = \varphi_i$.

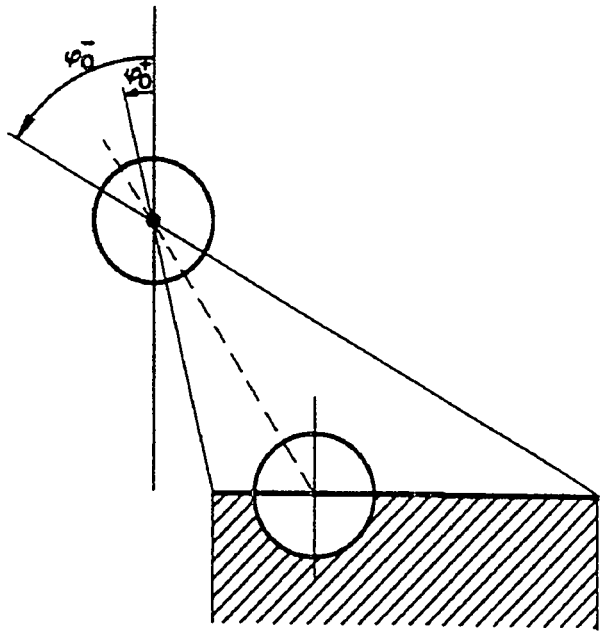


Figure F4.2.5b Minimum and maximum angles subtended by a flat finite surface as seen from the detector site

The integral defined by Eq. (F4.2.14) is then evaluated as

$$\phi_D = 2\pi \sum_{i=1}^{N} f_{C\gamma_i} \psi_S(\mu_{\gamma_i}) \Delta\mu_{\gamma_i} = 2\pi \left[\frac{\cos(\varphi_0^+) - \cos(\varphi_0^-)}{N} \right] \sum_{i=1}^{N} f_{C\gamma_i} \psi_S(\mu_{\gamma_i}) \ . \qquad \text{(F4.2.16a,b)}$$

Knowing $\mu_{\gamma_i} = \cos(\gamma_i)$, and knowing the surface flux in certain discrete directions $\{\psi(\mu_m, r_S), m=1,...,MM\}$, we need only decide what value to assign $\psi_S(\mu_{\gamma_i})$ at each point (i=1,...,N). Dividing the unit sphere into discrete bands as shown in Fig. F4.2.3 (where the outward-directed normal at the surface, $\underset{\sim}{a}_x$, is parallel to $\underset{\sim}{r}$), XSDOSE then assigns $\psi_S(\mu_{\gamma_i})$ the value of the angular flux (ψ_m) whose associated range (μ_m^-, μ_m^+) includes μ_{γ_i}.

F4.2.2.2 Determination of $\cos(\varphi_0^+)$, $\cos(\varphi_0^-)$, and $f_{C\gamma}$ for Detector Points Located Some Distance From a Flat Circular Disc (Representing the End of a Cylinder)

Expressions for the minimum and maximum angles subtended by a flat circular disc of radius R as seen from a detector located x cm above the plane of the disc at $r = \sqrt{y_D^2 + z_D^2}$ may be written easily after inspection of Fig. F4.2.6. Obviously, if the detector is located above any portion of the disc (r = 0, 0<r<R, r = R), the minimum angle subtended by the disc is $\varphi_0^+ = 0°$ [in which case $\cos(\varphi_0^+) = 1.0$]. If the point is located off to the side of the disc (r>R), as shown in Fig. F4.2.6d, then

$$\varphi_0^+ = \arctan\,[(r-R)/x] \ , \qquad r>R \qquad \text{(F4.2.17a)}$$

and

$$\cos\,\varphi_0^+ = x/\sqrt{x^2 + (r-R)^2} \ , \qquad r>R \ . \qquad \text{(F4.2.17b)}$$

In each case, the maximum angle subtended by the disc is given by

$$\varphi_0^- = \arctan\,[(r+R)/x] \ , \qquad r\geq 0 \qquad \text{(F4.2.18a)}$$

with

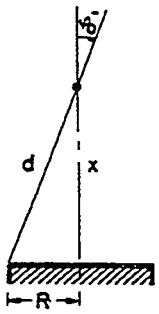
$$\cos\,\varphi_0^- = x/\sqrt{x^2 + (r+R)^2} \ , \qquad r\geq 0 \ . \qquad \text{(F4.2.18b)}$$

Knowing the range of integration $[\cos(\varphi_0^-) < \mu_\gamma < \cos(\varphi_0^+)]$, Eq. (F4.2.14) may then be evaluated numerically by breaking the range into N discrete intervals [cf. Eq. (F4.2.16)]. As noted previously, each discrete interval ($\Delta\mu_{\varphi_i}$) has a characteristic angle ($\varphi_i = \gamma_i$) such that, when projected onto the plane containing the source, each interval appears as a narrow circular band [represented in Fig. F4.2.7a as the circular line, C_i]. In each case (I = 1,...,N), we must determine what fraction ($f_{C\gamma_i}$) of that narrow circular band overlaps the flat disc-shaped surface source (S).

To determine $f_{C\gamma_i}$, let us consider the plane (x = 0) containing the flat disc-shaped source (representing the end of a cylinder). In the (y,z) plane, the boundary of the finite disc (S) may be described as

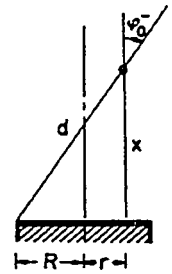
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(a)



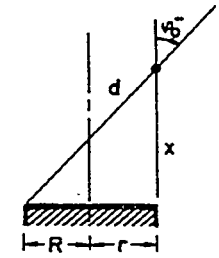
$$\begin{cases} \varphi_o^+ = 0^\circ \\ \varphi_o^- = \arctan\,[(r+R)/x]\ ,\ r=0 \\ \cos\,\varphi_o^+ = 1.0 \\ \cos\,\varphi_o^- = x/d = x/\sqrt{x^2 + (r+R)^2}\ ,\ r=0 \end{cases}$$

(b)



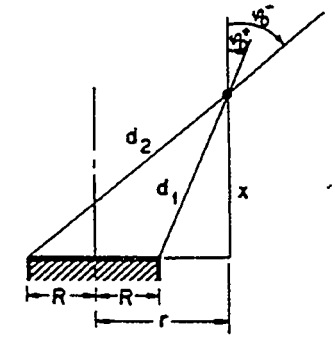
$$\begin{cases} \varphi_o^+ = 0^\circ \\ \varphi_o^- = \arctan\,[(r+R)/x] \\ \cos\,\varphi_o^+ = 1.0 \\ \cos\,\varphi_o^- = x/d = x/\sqrt{x^2+(r+R)^2} \end{cases}$$

(c)



$$\begin{cases} \varphi_o^+ = 0^\circ \\ \varphi_o^- = \arctan\,[(r+R)/x]\ ,\ r=R \\ \cos\,\varphi_o^+ = 1.0 \\ \cos\,\varphi_o^- = x/d = x/\sqrt{x^2+(r+R)^2}\ ,\ r=R \end{cases}$$

(d)



$$\begin{cases} \varphi_o^+ = \arctan\,[(r-R)/x] \\ \varphi_o^- = \arctan\,[(r+R)/x] \\ \cos\,\varphi_o^+ = x/d_1 = x/\sqrt{x^2+(r-R)^2} \\ \cos\,\varphi_o^- = x/d_2 = x/\sqrt{x^2+(r+R)^2} \end{cases}$$

Figure F4.2.6 Minimum and maximum angles subtended by a flat circular disc as seen from various points

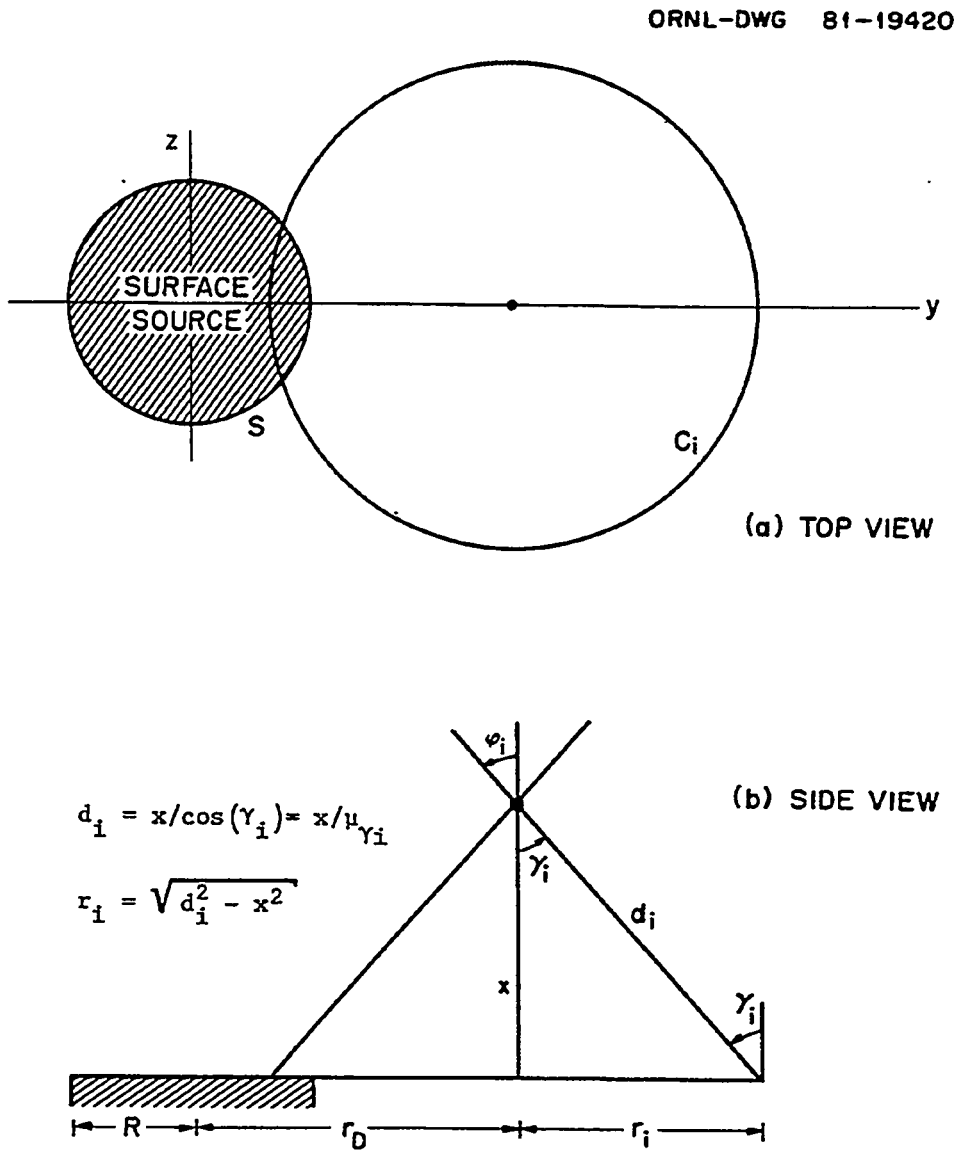


Figure F4.2.7 Sketch showing (a) one way that an arbitrary circular line [C_i] may overlap a flat, disc-shaped source, and (b) how, given the polar angle φ_i, one can calculate the radius of the corresponding circle [r_i] in the yz plane

$$\text{DISC(S):}\quad y^2 + z^2 = R^2, \tag{F4.2.19}$$

where R is the radius of the disc. Likewise, the circle C_i may be described as

$$\text{CIRCLE}(C_i):\quad (y - r_D)^2 + z^2 = r_i^2, \tag{F4.2.20}$$

where r_D is the location of the detector in the y,z plane ($r_D^2 = y_D^2 + z_D^2$), and r_i is the radius of circle (C_i) corresponding to the discrete angle γ_i. As shown in Fig. F4.2.7b,

$$r_i = x \tan(\gamma_i) = x\sqrt{(1/\mu_{\gamma_i})^2 - 1}\ . \tag{F4.2.21a,b}$$

To determine the extent of any possible overlap, let us consider the situation at $z = 0$, where the disc is bounded by

$$\text{DISC(S):}\quad y_{1S} \le y \le y_{2S},\quad y_{1S} = -R,\quad y_{2S} = +R \tag{F4.2.22}$$

and the circle (C_i) is bounded by

$$\text{CIRCLE}(C_i):\quad y_{1C} \le y \le y_{2C},\ y_{1C} = r_D - r_i,\ y_{2C} = r_D + r_i\ . \tag{F4.2.23}$$

As shown in Fig. F4.2.8, there are four possibilities:

(1) if $y_{1S} < y_{1C} < y_{2C} < y_{2S}$, the circle ($C_i$) lies entirely within S, and $f_{C\gamma_i} = 1$ (cf. Fig. F4.2.8a);

(2) if $y_{1S} < y_{2S} < y_{1C} < y_{2C}$, the circle ($C_i$) lies entirely outside S and $f_{C\gamma_i} = 0$ (cf. Fig. F4.2.8b);

(3) if $y_{1C} < y_{1S} < y_{2S} < y_{2C}$, the circle ($C_i$) fully encloses S but the circular line itself never touches S, and $f_{C\gamma_i} = 0$ (cf. Fig. F4.2.8c);

(4) if $y_{1S} < y_{1C} < y_{2S} < y_{2C}$, the circle ($C_i$) partially overlaps S, and $f_{C\gamma_i}$ must be determined as shown below (cf. Fig. F4.2.8d and/or Fig. F4.2.9).

Given that $y_{1S} < y_{1C} < y_{2S} < y_{2C}$, we may determine the amount of overlap by computing the point of intersection (cf. Fig. F4.2.9). At the point of intersection, for example, we may subtract Eq. (F4.2.20) from Eq. (F4.2.19) to obtain

$$2yr_D - r_D^2 = R^2 - r_i^2, \tag{F4.2.24}$$

from which we obtain the point of intersection (y*):

$$y^* = (R^2 + r_D^2 - r_i^2)/2r_D\ . \tag{F4.2.25}$$

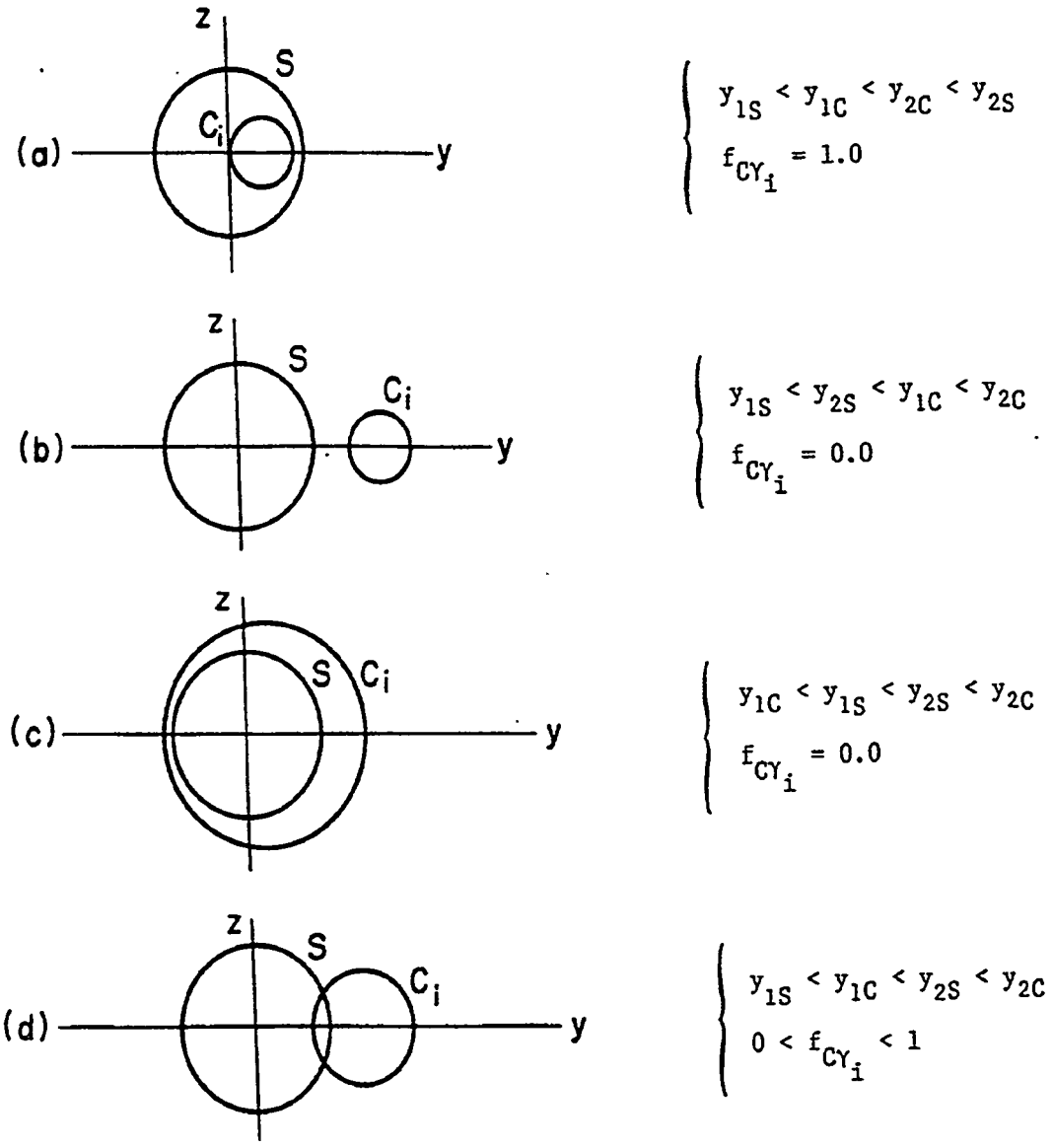


Figure F4.2.8 Different ways that an arbitrary circular line (C_i) may/may not overlap a disc-shaped surface (S). Here, y_1 and y_2 denote the left and right boundaries of the circle (C_i) and the surface (S); f_{CY_i} denotes the fraction of the circular line overlapping the finite surface

Referring to Fig. F4.2.9, the angle α may then be computed as

$$\alpha = \arccos[(r_D - y^*)/r_i] \ . \qquad \text{(F4.2.26)}$$

Knowing α, the fraction of the circular line (C_i) which lies on the disc-shaped surface (S) is then given by

$$f_{C\gamma_i} = \left(\frac{\alpha}{\pi}\right) \ . \qquad \text{(F4.2.27)}$$

F4.2.2.3 Determination of $\cos(\varphi_0^+)$, $\cos(\varphi_0^-)$, and $f_{C\gamma}$ for Detector Points Located Some Distance From a Flat Rectangular Surface Source of Finite Extent

As shown in Fig. F4.2.5, each angle φ_i ($\varphi_i = \gamma_i = \arccos \mu_{\gamma i}$) corresponds to a circle (C_i) in the plane containing the finite rectangular source. If we let r_i denote the radius of that circle in the yz plane (at $x = 0$), then

$$\cos \varphi_0^+ = x_D/\sqrt{x_D^2 + r_{min}^2} \qquad \text{(F4.2.28)}$$

and

$$\cos \varphi_0^- = x_D/\sqrt{x_D^2 + r_{max}^2}, \qquad \text{(F4.2.29)}$$

where r_{min} and r_{max} denote the radii of the smallest and largest circles intersecting any point on the finite rectangular surface ($y_1 \le y \le y_2$; $z_1 \le z \le z_2$). If the detector is located at (x_D y_D z_D), then r_{max} will inevitably be the distance from (y_D, z_D) to one of the four corners of the finite surface: (y_1, z_1), (y_1, z_2), (y_2, z_1), or (y_2, z_2). Denoting each of these distances as r_A, r_B, r_C, and r_D, r_{max} may then be defined as

$$r_{max} = \max\{r_A, r_B, r_C, r_D\} \ . \qquad \text{(F4.2.30)}$$

To determine r_{min}, one must consider the position of (y_D, z_D) relative to the finite surface in the yz plane. In Fig. F4.2.10, for example, the surface (S) is assumed to lie between $y_1 = 0$ and $y_2 = y_{max}$, and between $z_1 = 0$ and $z_2 = z_{max}$. Obviously, if the detector is located directly above some point on the finite surface ($y_1 \le y_D \le y_2$; $z_1 \le z_D \le z_2$), then $r_{min} = 0$ and $\cos \varphi_0^+ = 1.0$. If (y_D, z_D) lies in any of the other unshaded regions of Fig. F4.2.10, then

$$r_{min} = \max\{(y_1 - y_D), (y_D - y_2), (z_D - z_2), (z_1 - z_D)\} \ . \qquad \text{(F4.2.31a)}$$

Lastly, if (y_D, z_D) lies in any of the shaded regions of Fig. F4.2.10, then

$$r_{min} = \min\{r_A, r_B, r_C, r_D\} \ , \qquad \text{(F4.2.31b)}$$

where r_A, r_B, r_C, and r_D denote the distance from (y_D, z_D) to each of the four corners of the finite surface (S).

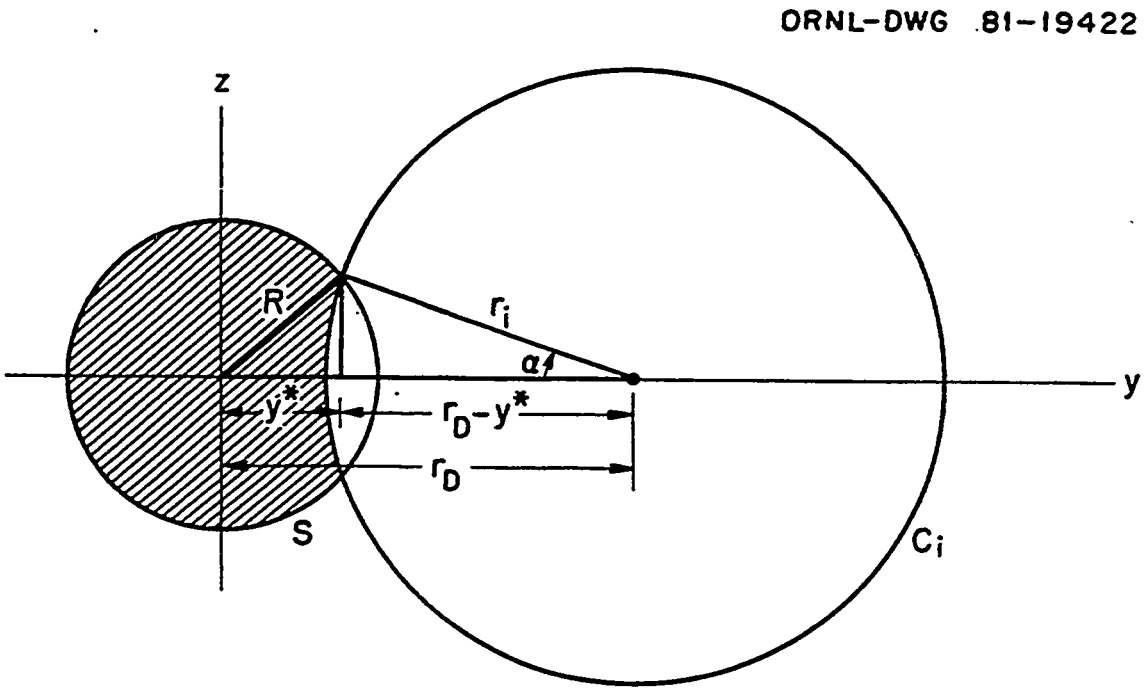


Figure F4.2.9 Sketch used to determine the point of intersection (y*) and the amount of overlap [$f_{C\gamma_i} = \alpha/\pi$] between an arbitrary circular line (C_i) and a disc-shaped surface (S) of radius R

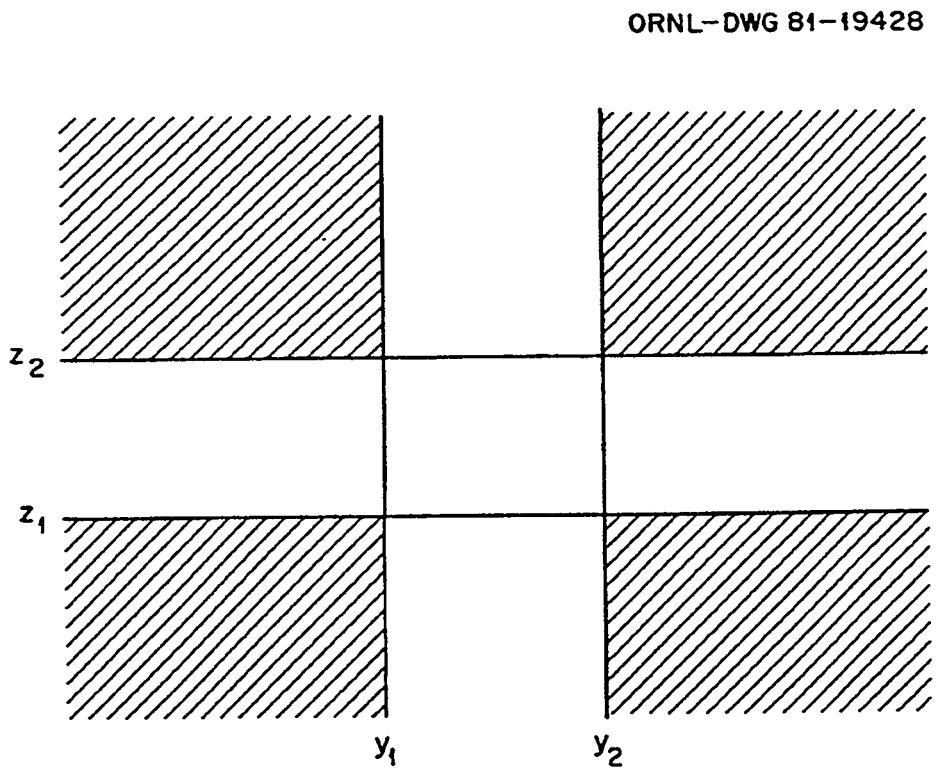


Figure F4.2.10 Different regions in the yz plane surrounding the finite rectangular surface bounded by y_1, y_2, z_1, and z_2

Knowing the range of integration [$\cos(\varphi_0^-) < \mu_\gamma < \cos(\varphi_0^+)$], Eq. (F4.2.14) may then be evaluated numerically by breaking the range into N discrete intervals [cf. Eq. (F4.2.16)]. As noted previously, each discrete interval ($\Delta\mu_{\varphi_i}$) has a characteristic angle ($\varphi_i = \gamma_i$) such that, when projected onto the plane containing the rectangular surface, each interval appears as a narrow circular band (represented in Fig. F4.2.5a as the circular line, C_i). In each case (i=1,...,N), we must determine what fraction ($f_{C\gamma_i}$) of that narrow circular band overlaps the finite surface (S) defined by $y_1 \le y \le y_2$, $z_1 \le z \le z_2$. Depending on the size and shape of the rectangular surface, the size of the circle (r_i), and the location of the circle relative to the surface, the two may overlap in a great variety of different ways! Fortunately, however, the fraction of each circle overlapping the finite rectangular surface can be determined quite easily by first finding the points of intersection ($C_i \cap S$) and then checking the location of a single intermediate point along each arc of the circle.

The procedure described above for determining f_{CY_i} is most easily carried out in a translated coordinate system defined by

$$u = y - y_D \,, \tag{F4.2.32a}$$

$$v = z - z_D \,. \tag{F4.2.32b}$$

The center of the circle is thus situated at the origin of the new coordinate system, as shown in Fig. F4.2.11. The circle (C_i) is then defined by

$$u^2 + v^2 = (r_i)^2 \,, \tag{F4.2.33}$$

and the rectangular surface (S) is bounded by the four lines

$$u_1 = -y_D \tag{F4.2.34a}$$

$$u_2 = y_{max} - y_D \tag{F4.2.34b}$$

$$v_1 = -z_D \tag{F4.2.34c}$$

$$v_2 = z_{max} - z_D \,. \tag{F4.2.34d}$$

Substituting Eq. (F4.2.34a) into Eq. (F4.2.33) may yield one or two points of intersection, or none at all. Likewise, substitution of Eq. (F4.2.34b) into Eq. (F4.2.33) may yield 0, 1, or 2 points of intersection; substitution of Eq. (F4.2.34c) may yield 0, 1, or 2 points of intersection; and substitution of Eq. (F4.2.34d) may yield 0, 1, or 2 points of intersection. Altogether, we may have as many as 8 points of intersection, or as few as 0. Let J denote the total number of intersections found in this fashion. If $J \leq 1$, the circle C_i may lie totally outside the rectangular surface (S), it may fully enclose the rectangular surface, or it may lie entirely within the rectangular surface. After checking the location of any arbitrary point on the circle (say $u = 0$, $v = r_i$), f_{CY_i} would then be assigned a value of 0.0 or 1.0. If $J \geq 2$, we must pursue the matter just a little further. Knowing the coordinates of the various points of intersection $[(u_j, v_j), j=1,\ldots,J]$, we may number them in a counterclockwise direction and compute the polar angle (α) associated with each, so that they can now be described as $[(r_i, \alpha_j), j=1,\ldots,J]$. Defining (r_i, β_j) as the midpoint along each of the arcs, we can now check the location of $(u_j^* = r_i \cos\beta_j, v_j^* = r_i \sin\beta_j)$ to determine whether the particular arc lies on the rectangular surface (S) or external to it; if it lies on the surface, we set a flag (d_j) equal to 1.0, and if it lies outside the region we set d_j equal to zero. The fraction of the circular line lying on the finite rectangular surface is then given by

$$f_{CY_i} = \left(\frac{1}{2\pi}\right) \left\{ d_1[\alpha_1 + (2\pi - \alpha_j)] + \sum_{j=1}^{J-1} d_j (\alpha_{j+1} - \alpha_j) \right\}. \tag{F4.2.35}$$

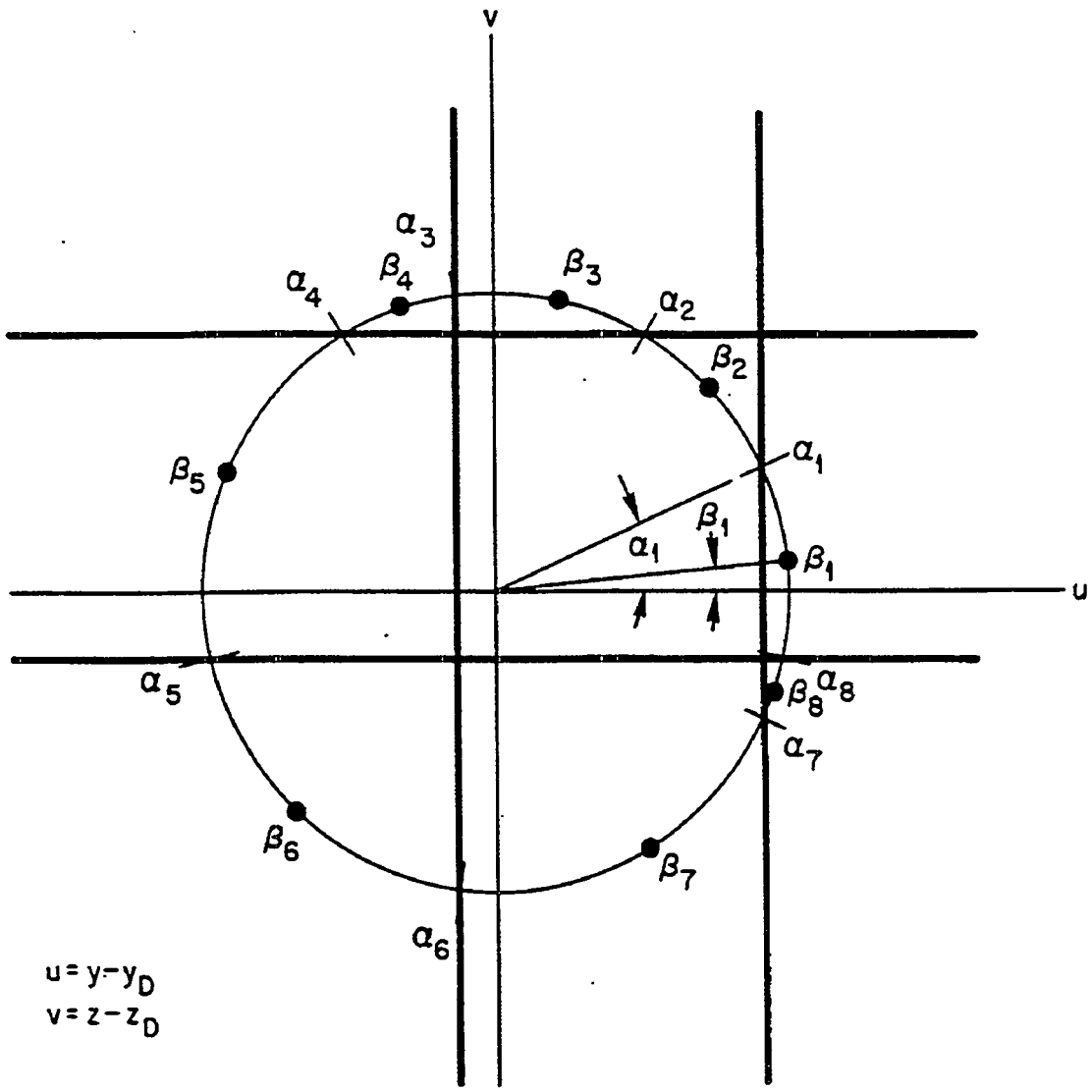


Figure F4.2.11 Sketch used to illustrate how one can determine what fraction (f_{CY_i}) of an arbitrary circular line (C_i) overlaps a finite rectangular surface (S). In the translated coordinate system shown here, $u = y - y_D$ and $v = z - z_D$, such that the circle (C_i) now appears centered at the origin of the uv plane, and the rectangular surface bounded by $y_1 = 0$, $y_2 = y_{max}$, $z_1 = 0$, $z_2 = z_{max}$ now appears to be shifted somewhat. The intersection(s) of these boundary lines with the circle are designated as $\{\alpha_j; j = 1,2,...,J; 0 \le J \le 8\}$, and the midpoints of the resulting arcs are designated as $\{\beta_j; j = 1,2,...,J; 0 \le J \le 8\}$.

F4.2.3 CALCULATION OF THE SCALAR FLUX AT POINTS SOME DISTANCE FROM A FINITE CYLINDRICAL SOURCE

F4.2.3.1 Pertinent Characteristics of Discrete-Ordinate Quadrature Sets in Cylindrical Geometry

In cylindrical geometry, the angular flux at any point $[\psi(\underset{\sim}{r}, \underset{\sim}{\Omega})]$ must be described in terms of two angular variables, μ and η, where $\eta = \cos\theta$ is the direction cosine of $\underset{\sim}{\Omega}$ with respect to the z axis and $\mu = \cos\varphi$ is the direction cosine of $\underset{\sim}{\Omega}$ with respect to the outward-directed normal ($\underset{\sim}{a}_r$). To calculate the scalar flux at any point within the system (or on the surface of the cylinder), XSDRNPM takes a weighted sum of the angular fluxes (ψ_m) in each of the various directions ($\underset{\sim}{\Omega}_m$) associated with the given quadrature $\{w_m; \eta_m, \mu_m\}$:

$$\phi = \sum_{m=1}^{MM} w_m \psi_m = \sum_{m=1}^{MM} w_m \psi(r,\eta_m,\mu_m) . \qquad \text{(F4.2.36)}$$

Even though the direction cosines and quadrature weights are predetermined by XSDRNPM in a way that ensures accurate determination of the first N moments of the angular flux,* the weights may (in a simplistic sense) be viewed as the solid angle over which the corresponding angular flux is considered constant $[\psi(\eta,\mu) \doteq \psi(\eta_m, \mu_m)]$.** Figure F4.2.12 shows the angular directions corresponding to an S_6 quadrature in cylindrical geometry. In XSDOSE, as in XSDRNPM, the quadrature is assumed to have certain characteristic features. These features are summarized in Table F4.2.1. If ISN denotes the order of the quadrature, the number of "eta levels" is given by

$$L = ISN/2 , \qquad \text{(F4.2.37)}$$

and the total number of discrete directions (MM) is given by

$$MM = ISN*(ISN + 4)/4 . \qquad \text{(F4.2.38)}$$

For our purposes, all discrete directions $\{\eta_m, \mu_m\}$ having the same polar angle (θ) are said to comprise a given "eta level." The width of each "eta level" will be of interest later.

If $\ell = 1$ denotes the eta level with the smallest value of θ, and $\ell = L$ denotes the eta level with the largest value of $\theta(\theta < 90°)$, then

---

*Given the order of the quadrature (ISN), XSDRNPM and XSDOSE both follow the same procedure for determining the direction cosines (η_m, μ_m) and quadrature weights (w_m). See Sect. M7.2.5.7 for additional details.

**This simplistic scheme for determining η_m^-, η_m^+, φ_m^-, and φ_m^+ is somewhat arbitrary. Note, for example, that one could specify a quadrature set in which η_m or μ_m fall outside the angular range defined by $(\eta_m^-, \eta_m^+, \varphi_m^-, \varphi_m^+)$. That, however, is very rarely the case. Indeed, the scheme proposed here for determining $(\eta_m^-, \eta_m^+, \varphi_m^-, \varphi_m^+)$ and subsequently assigning $\psi(\eta, \varphi_i, r_s)$ some value $[\psi_m(r_s)]$ based on η and φ_i is no more arbitrary than other schemes that have been proposed. In addition, the present scheme allows XSDOSE to faithfully reproduce the scalar fluxes calculated by XSDRNPM whenever the detector point (r_D) is arbitrarily close to the surface (r_S).

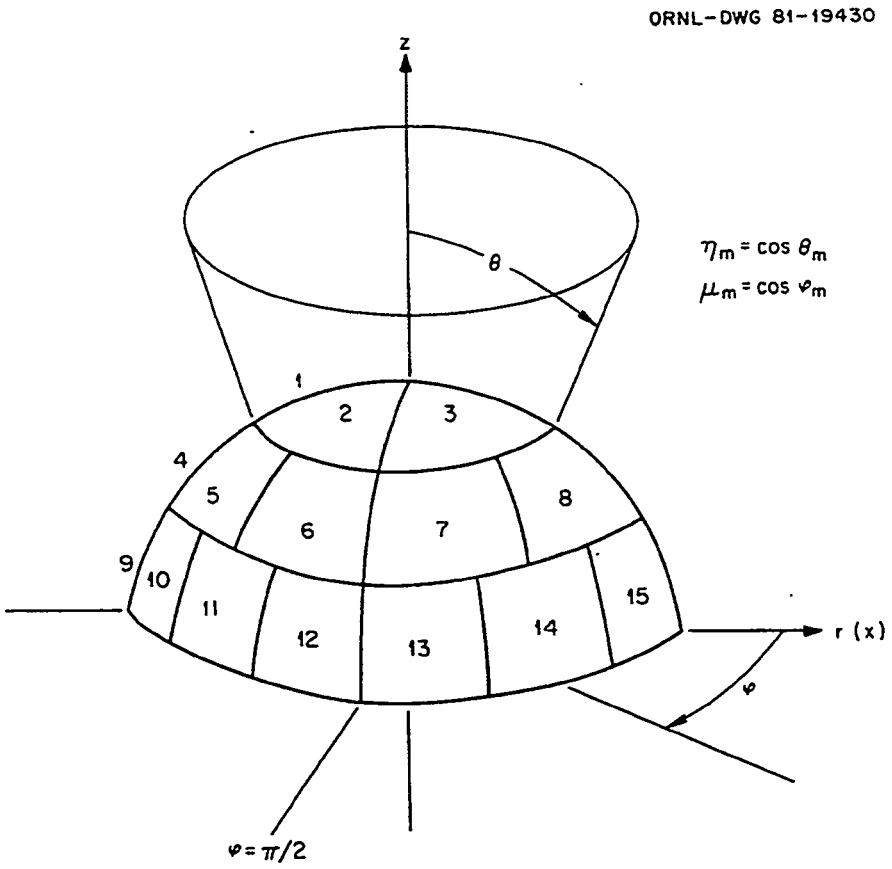


Figure F4.2.12 Relationship between the spatial coordinates in cylindrical geometry (r,z) and each of the corresponding quadrature directions $\{\underset{\sim}{\Omega}(\theta_m, \varphi_m)$; m=1,2,...,MM; MM=ISN*(ISN+4)/4$\}$. (Here, ISN=6 and MM=15.)

Table F4.2.1 Characteristics of cylindrical quadrature sets generated by XSDRNPM and/or "assumed" by XSDOSE (cf. Fig. F4.2.12)

(1) The number of quadrature points used is MM = ISN*(ISN + 4)/4.

(2) The number of "eta levels" is L = ISN/2.

(3) $\mu_1\ \mu_4\ \mu_9\ \mu_{16} \ldots\ \mu_K$ represent the first discrete direction in each eta level ($K = L^2$).

(4) A quadrature weight of zero is assigned to the first discrete direction in each eta level (i.e., $w_1 = w_4 = w_9 = w_{16} = \ldots = w_K = 0$).

(5) The eta levels are arranged such that
$\mu_K < \mu_J < \ldots < \mu_{16} < \mu_9 < \mu_4 < \mu_1 < 0$ [$K = L^2$, $J = (L-1)^2$].

(6) Half of the discrete directions in each eta level are inward-directed, while the other half are outward-directed:

$\mu_1 < \mu_2 < 0 < \mu_3$
$\mu_4 < \mu_5 < \mu_6 < 0 < \mu_7 < \mu_8$
$\mu_9 < \mu_{10} < \mu_{11} < \mu_{12} < 0 < \mu_{13} < \mu_{14} < \mu_{15}$
$\mu_{16} < \mu_{17} < \mu_{18} < \mu_{19} < \mu_{20} < 0 < \mu_{21} < \mu_{22} < \mu_{23} < \mu_{24}$

(7) Except for the first discrete direction, all the others in a given eta level are assigned the same quadrature weight:

$w_1 = 0;\ w_2 = w_3$
$w_4 = 0;\ w_5 = w_6 = w_7 = w_8$
$w_9 = 0;\ w_{10} = w_{11} = w_{12} = w_{13} = w_{14} = w_{15}$
$w_{16} = 0;\ w_{17} = w_{18} = w_{19} = w_{20} = w_{21} = w_{22} = w_{23} = w_{24}$

(8) $\sum_{i=1}^{MM} w_i = 1.0$ and $\sum_{i=1}^{MM} w_i\mu_i = 0.0$.

(1) the first discrete direction in each eta level (corresponding to μ_m, $m = \ell^2$) will be located at $\varphi = \pi$ and have a weight (w_m) of zero;

(2) of the remaining discrete directions in the given eta level (ℓ), ℓ will be inward-directed and ℓ will be outward-directed, as shown in Fig. F4.2.12;

(3) with the exception of the first discrete direction which has a weight of zero, all the other discrete directions in a given eta level are assigned the same weight;

(4) the upper and lower limits for each eta level (ℓ) are defined by

$$\eta_1^+ = 1.0 \ , \ \eta_1^- = 1 - 2w_2 \qquad \text{(F4.2.39a,b)}$$

$$\eta_\ell^+ = \eta_{\ell-1}^- \ , \ \ell \geq 2 \qquad \text{(F4.2.39c)}$$

$$\eta_\ell^- = \eta_\ell^+ - 2\ell w_j \text{ where } j = \ell^2 + 1 \text{ and } \ell \geq 2 \qquad \text{(F4.2.39d)}$$

(5) the upper and lower limits for each azimuthal angle (m) in a given eta level (ℓ) are defined by

$$\varphi_m^+ = \pi \quad , \varphi_m^- = \varphi_m^+ - \left(\frac{\pi}{2\ell}\right) \quad , m = \ell^2 + 1 \qquad \text{(F4.2.40a,b)}$$

$$\varphi_m^+ = \varphi_{m-1}^- \quad , \phi_m^- = \phi_m^+ - \left(\frac{\pi}{2\ell}\right) \quad , \ell^2 + 2 \leq m \leq (\ell + 1)^2 - 1 \ . \qquad \text{(F4.2.40c,d)}$$

F4.2.3.2 Use of Symmetry to Decompose the General Problem (at Any Detector Point) Into Several Parts, Each Having the Same Standard Form

From Fig. F4.2.12, we note that all of the discrete angular directions used in the XSDRNPM calculation lie in a single quadrant of the unit sphere. Because the cylindrical body is assumed to be infinitely long in the XSDRNPM calculation, the downward-directed angular fluxes would be symmetric with respect to the upward-directed angular fluxes, and one would have $\psi(\underset{\sim}{r},\theta = \pi - \theta_0,\varphi) = \psi(\underset{\sim}{r},\theta = \theta_0,\varphi)$. Hence, downward-directed quadrature points were unnecessary. In a typical XSDOSE calculation, however, one may need to determine the scalar flux at a point (r_D, z_D) which is either above or below the midplane of a finite cylinder (cf. Fig. F4.2.13a or Fig. F4.2.13b). In either case, some particles reaching the detector left the cylindrical surface traveling in a downward direction and some of the particles left the cylindrical surface traveling in an upward direction. If the detector point is not at the midplane, the two contributions will not be equal. To obtain the desired result, the cylindrical surface shown in Fig. F4.2.13a (or Fig. F4.2.13b) is broken into two smaller cylindrical surfaces h_1 and h_2, both of which are located below the detector. The total scalar flux at the detector is then evaluated in terms of the upward-directed angular flux components leaving the two surfaces, h_1 and h_2, that is

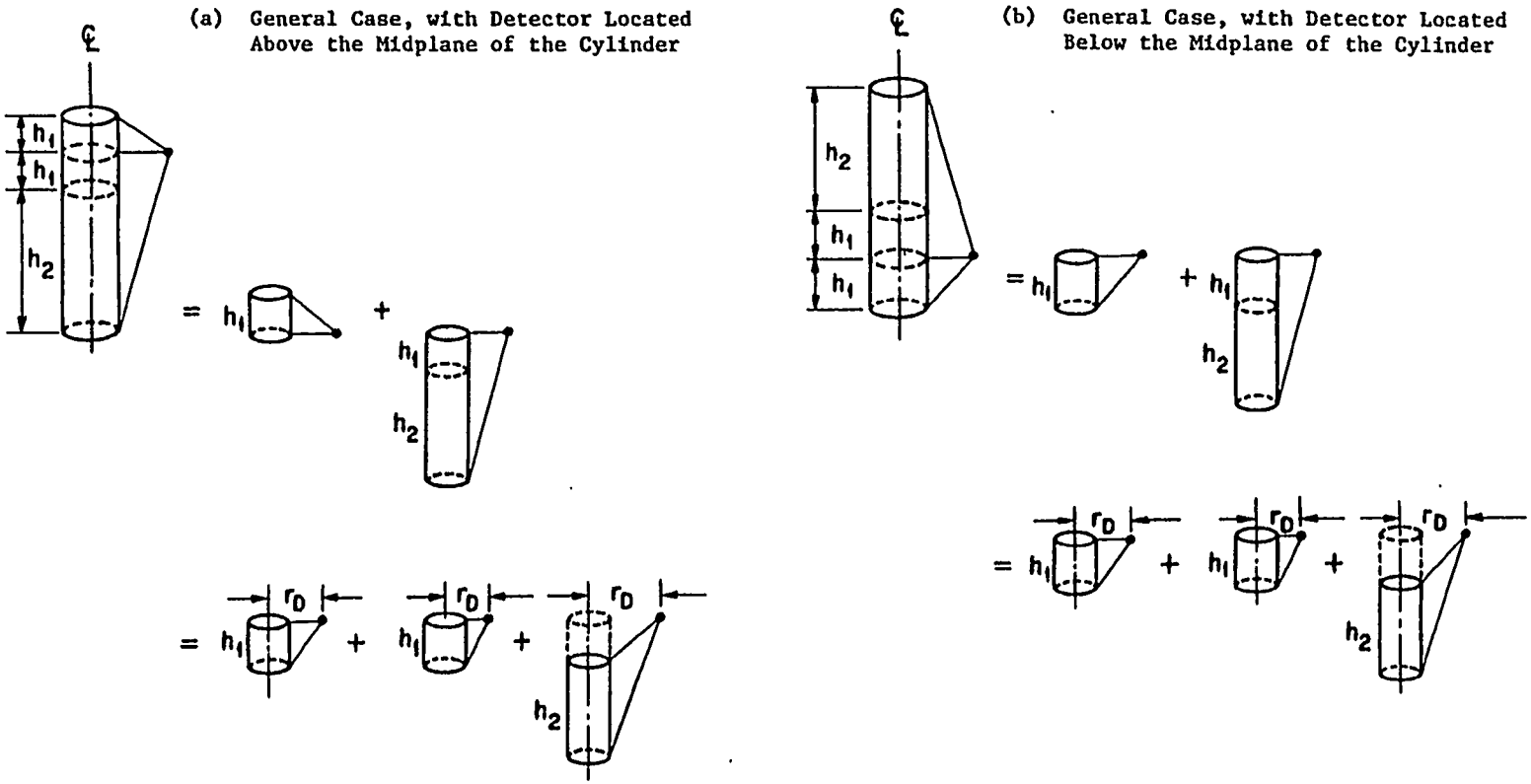


Figure F4.2.13 Use of symmetry to decompose the general problem (with a detector located either above or below the midplane of a cylinder) into several parts, each having a shorter cylindrical surface located below the plane of the detector

$$\phi_D = \phi_D\Big|_{h_2} + 2\phi_D\Big|_{h_1} . \qquad \text{(F4.2.41)}$$

Lastly, we also note from Fig. F4.2.12 that all of the discrete angular directions used in the XSDRNPM calculation lie in that quadrant of the unit sphere wherein $0 \le \varphi \le \pi$. Because of the symmetry condition imposed by the 1-D cylindrical model, $\psi(\underset{\sim}{r}, \theta, -\varphi) = \psi(\underset{\sim}{r}, \theta, \varphi)$. Hence the other angular directions ($\pi < \varphi < 2\pi$) would have been superfluous. In the XSDOSE calculation for the scalar flux, we account for this by integrating the outward-directed angular flux [$\psi(\underset{\sim}{r}, \theta, \varphi)$] from $\varphi = 0$ to $\varphi = \varphi_{max}$ ($\varphi_{max} \le 90°$) and doubling the final result. Thus, for example,

$$\phi_D\Big|_{h_2} + \int \psi(\underset{\sim}{r}_D, \underset{\sim}{\Omega}) d\underset{\sim}{\Omega} = \int_0^{2\pi} \int_{\theta_{min}}^{\theta_{max}} \psi(\underset{\sim}{r}_D \theta, \varphi) \sin\theta d\theta \, d\varphi$$

$$= 2\int_0^{\varphi_{max}} \int_{\theta_{min}}^{\theta_{max}} \psi(\underset{\sim}{r}_D, \theta, \varphi) \sin\theta d\theta \, d\varphi . \qquad \text{(F4.2.42)}$$

F4.2.3.3 Actual Equations Used to Calculate the Contribution From a Cylindrical Surface Source of Finite Length

To determine the scalar flux at any arbitrary point (r_D, z_D) some distance from a finite cylindrical source ($r = r_s$, $0 \le z \le L$), XSDOSE may break the surface into two separate pieces as shown in Figs. F4.2.13a and F4.2.13b. For the purpose of this discussion, we will consider only the contribution from one of the component parts, as illustrated in Fig. F4.2.14. To determine the scalar flux, XSDOSE numerically integrates what appears to be the angular flux at the point of interest:

$$\phi_D = \int \psi(\underset{\sim}{\Omega}, r_D, z_D) d\underset{\sim}{\Omega} = \int\int \psi(\theta, \varphi, r_D, z_D) \sin\theta d\theta d\varphi \qquad \text{(F4.2.43a,b)}$$

$$= 2\int_0^{\varphi_0} \left[\int_{\theta_\varphi^-}^{\theta_\varphi^+} \psi(\theta, \varphi, r_D, z_D) \sin\theta d\theta \right] d\varphi = 2\int_0^{\varphi_0} £(\varphi) d\varphi , \qquad \text{(F4.2.43c,d)}$$

where

$$£(\varphi) = \int_{\theta_\varphi^-}^{\theta_\varphi^+} \psi(\theta, \varphi, r_D, z_D) \sin\theta d\theta \qquad \text{(F4.2.44)}$$

denotes the integral of ψ over a line on the surface of the cylinder, as defined by the angle φ. Note that this line will, of course, be parallel to the z-axis.

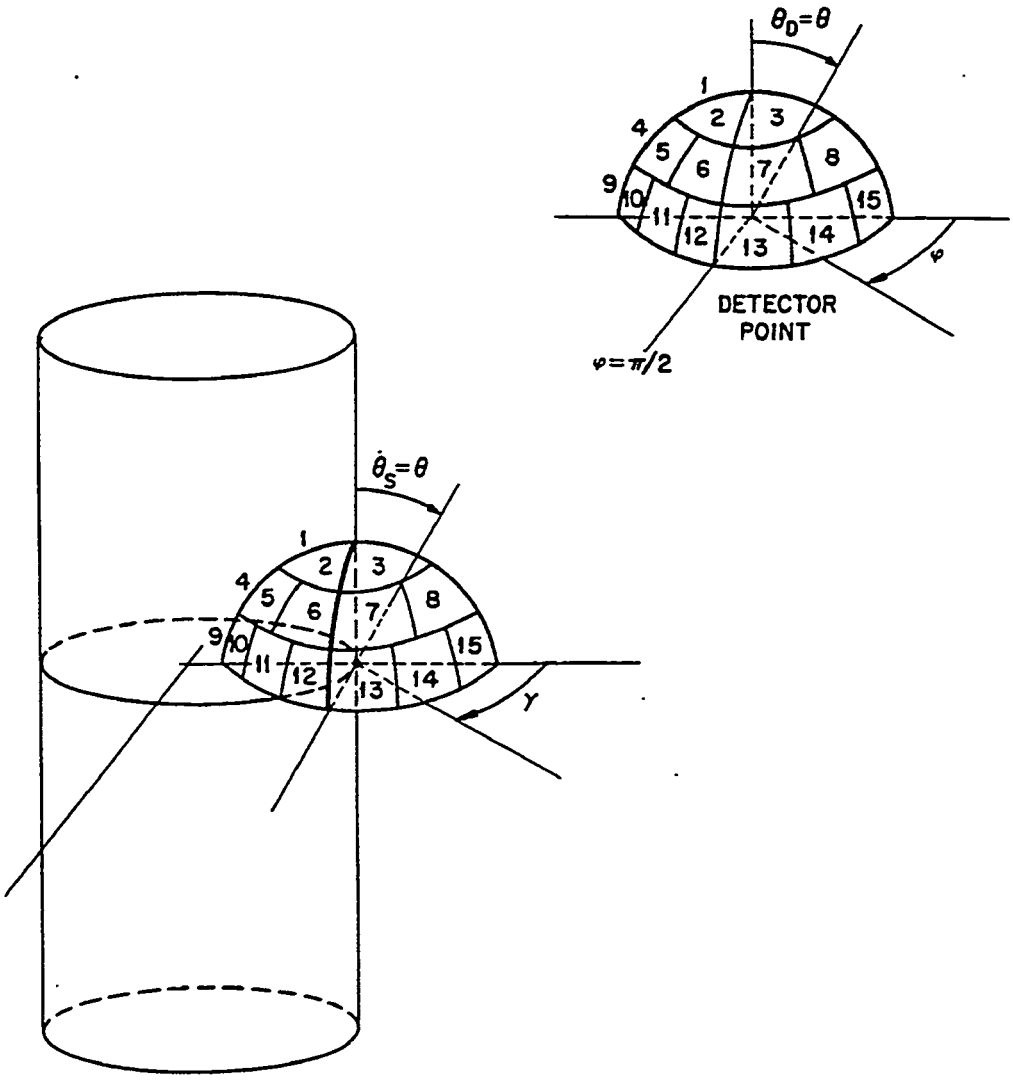


Figure F4.2.14 Lateral view of a cylindrical source and a point detector which shows the physical relationship between the angular flux components at the detector point $[\psi(\underset{\sim}{r}_D, \underset{\sim}{\Omega}_m(\theta_D,\varphi))]$ and the angular flux components at an arbitrary point on the surface of the cylinder $[\psi(\underset{\sim}{r}_s, \underset{\sim}{\Omega}_m(\theta_s,\gamma))]$

To define the various parameters somewhat more clearly, consider a "top view" of Fig. F4.2.14 as shown in Fig. F4.2.15. Obviously the maximum azimuthal angle (φ_0) subtended by the cylinder as seen from the detector point occurs when $\gamma = 90°$ and

$$\varphi_0 = \arcsin\left(\frac{r_S}{r_D}\right) . \qquad \text{(F4.2.45)}$$

Equation (F4.2.43) is then evaluated numerically by breaking the range of integration $0 < \varphi < \varphi_0$ into N equal intervals (specified in the input data as NINCRM; typically ~200). Denoting the upper and lower bounds of each interval as φ_i^+ and φ_i^-, the characteristic angle for each interval is defined as

$$\varphi_i = 0.5[\varphi_i^+ + \varphi_i^-] . \qquad \text{(F4.2.46)}$$

The integral defined by Eq. (F4.2.43d) is then evaluated as

$$\phi_D = 2\left(\frac{\varphi_0}{N}\right) \sum_{i=1}^{N} (\varphi_i) . \qquad \text{(F4.2.47)}$$

From Fig. F4.2.15a we see that those neutrons that fly past the detector at a fixed azimuthal angle (φ_i) are the same ones that left the surface of the cylinder making an angle γ_i relative to $\underset{\sim}{r}_S$, that is,

$$\psi(\theta, \varphi_i, \underset{\sim}{r}_D) = \psi(\theta, \gamma_i, \underset{\sim}{r}_S) . \qquad \text{(F4.2.48)}$$

To determine the angle γ_i corresponding to φ_i, we first apply the Law of Sines to determine the complementary angle β (cf. Fig. F4.2.15b). Recognizing that β is greater than 90°, we can then write

$$\gamma_i = \arcsin\left[\left(\frac{r_D}{r_S}\right) \sin\varphi_i\right] . \qquad \text{(F4.2.49)}$$

The line integral defined by Eq. (F4.2.44) may then be written as

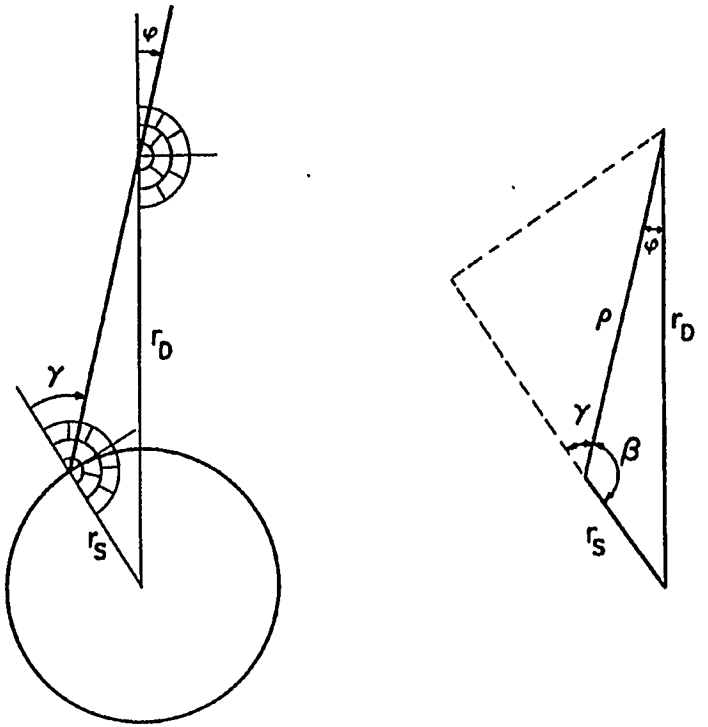
$$\pounds(\varphi_i) = \int_{\theta_{\varphi_i}^-}^{\theta_{\varphi_i}^+} \psi(\theta, \gamma_i, \underset{\sim}{r}_S) \sin\theta \, d\theta = \int_{\eta_{\varphi_i}^-}^{\eta_{\varphi_i}^+} \psi(\eta, \gamma_i, \underset{\sim}{r}_S) d\eta , \qquad \text{(F4.2.50a,b)}$$

where the limits of integration on the polar angle (θ) depend on the azimuthal angle φ_i. To determine those limits of integration, it is helpful to consider the lateral view of the cylinder and detector as shown in Fig. F4.2.16. If the finite cylinder extends from $z = 0$ to $z = h$ and the detector is located at $z = z_D$ ($z_D \geq h$)

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a) Physical relationship between φ and γ

b) Mathematical relationship between φ and γ



$$\frac{\sin \beta}{r_D} = \frac{\sin \varphi}{r_S}$$

$$\beta = \arcsin \left[\left(\frac{r_D}{r_S}\right) \sin \varphi\right] \qquad \beta \leq 90°$$

$$\beta = \pi - \arcsin \left[\left(\frac{r_D}{r_S}\right) \sin \varphi\right] \qquad \beta \geq 90°$$

$$\gamma + \beta = \pi$$

$$\gamma = \arcsin \left[\left(\frac{r_D}{r_S}\right) \sin \varphi\right] \qquad \varphi \leq 90°$$

Figure F4.2.15 Top view of a cylindrical source and a point detector that shows the physical and mathematical relationship between the azimuthal angular flux components at the detector point (angle φ) and the azimuthalangular flux components at the surface of the cylinder (angle γ)

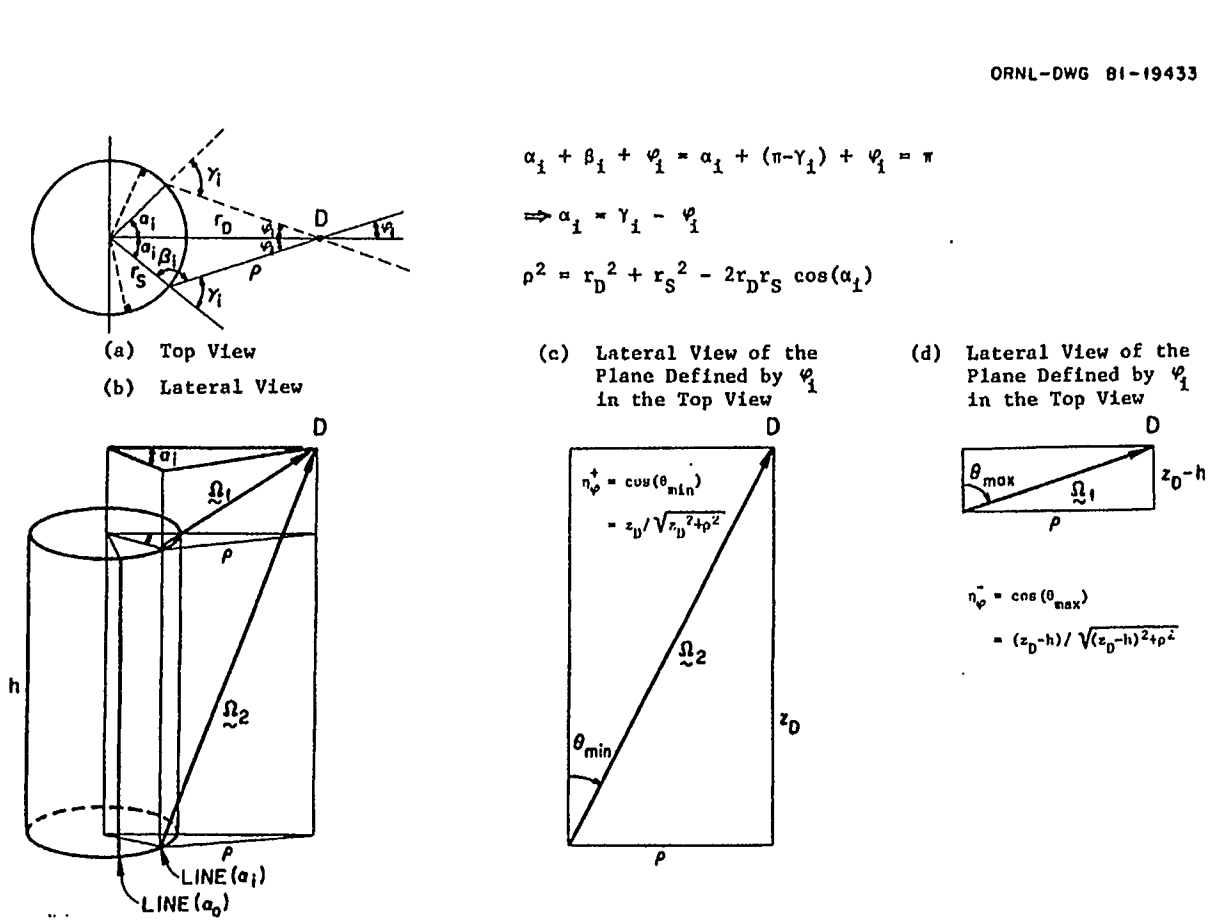


Figure F4.2.16 Lateral and top views of a cylindrical source and a point detector which show: (1) how to calculate the projected distance [ρ], in the XY-plane, from the detector to an arbitrary point on the surface of the cylinder; and (2) how to calculate the minimum and maximum polar angles [θ] subtended by the cylinder, in a plane defined by a specific azimuthal angle [ℓ] at the detector site

$$\eta^{+}_{\varphi_i} = \cos(\theta^{-}_{\varphi_i}) = z_D \Big/ \sqrt{z_D^2 + \rho^2} \qquad \text{(F4.2.51a)}$$

and

$$\eta^{-}_{\varphi_i} = \cos(\theta^{+}_{\varphi_i}) = (z_D - h) \Big/ \sqrt{(z_D - h)^2 + \rho^2}, \qquad \text{(F4.2.51b)}$$

where ρ, the projected distance in the xy plane from the detector to the cylinder, is determined by the angle φ_i; and is given by*

$$\rho^2 = r_D^2 + r_S^2 - 2r_D r_S \cos(\gamma_i - \varphi_i) \; . \qquad \text{(F4.2.51c)}$$

From the lateral view shown in Fig. F4.2.16b, it is clear that the plane defined by $\varphi = \varphi_i$ intersects the cylinder along a finite vertical line. Evaluation of the integral in Eq. (F4.2.50b) from $\eta^{-}_{\varphi_i}$ to $\eta^{+}_{\varphi_i}$ is therefore equivalent to evaluating the integral of ψ over the line defined by the intersection of the two surfaces. Evaluating the integral in terms of η is, however, somewhat more straightforward.

Evaluation of the line integral defined by Eq. (F4.2.50b) is direct and analytic. As a first step, let us break the range of integration into several "pieces," each corresponding to a different "eta level." If ISN denotes the order of the quadrature, the number of "eta levels" is given by L = ISN/2. If $\ell = 1$ denotes the eta level with the smallest value of θ, and $\ell = L$ denotes the eta level with the largest value of θ ($\theta \le 90°$), then the upper and lower limits for each eta level (ℓ) are defined by

$$\eta^{+}_1 = 1.0 \quad , \quad \eta^{-}_1 = 1 - 2w_2 \, , \qquad \text{(F4.2.52a,b)}$$

$$\eta^{+}_\ell = \eta^{-}_{\ell-1} \quad , \quad \ell \ge 2 \, , \qquad \text{(F4.2.52c)}$$

$$\eta^{-}_\ell = \eta^{+}_\ell - 2\ell w_j, \qquad \text{(F4.2.52d)}$$

where $j = \ell^2 + 1$ and $\ell \ge 2$.

The line integral defined by Eq. (F4.2.50b) can then be written as

$$\mathcal{E}(\varphi_i) = \int_{\eta^{-}_{\varphi_i}}^{\eta^{+}_{\varphi_i}} \psi(\eta, \gamma_i, \underset{\sim}{r}_S) d\eta = \sum_{\ell=1}^{L} \mathcal{E}_\ell(\varphi_i) \, , \qquad \text{(F4.2.53a,b)}$$

---

*This expression for ρ can be derived easily when one considers the "top view" of the cylinder and detector, as shown in Fig. F4.2.16a.

where the line integral over each of the individual eta levels [$\pounds_\ell(\varphi_i)$] is given by

$$\pounds_\ell(\varphi_i) = \begin{cases} = 0 & \text{if } \eta_\ell^+ < \eta_{\varphi_i}^- \text{ or } \eta_{\varphi_i}^+ < \eta_\ell^- \quad \text{(F4.2.54a)} \\ = \int_{\eta_\ell^-}^{\eta_\ell^+} \psi(\eta, \gamma_i, \underset{\sim}{r}_S) d\eta & \text{if } \eta_{\varphi_i}^- < \eta_\ell^- < \eta_\ell^+ < \eta_{\varphi_i}^+ \quad \text{(F4.2.54b)} \\ = \int_{\eta_{\varphi_i}^-}^{\eta_\ell^+} \psi(\eta, \gamma_i, \underset{\sim}{r}_S) d\eta & \text{if } \eta_\ell^- < \eta_{\varphi_i}^- < \eta_\ell^+ < \eta_{\varphi_i}^+ \quad \text{(F4.2.54c)} \\ = \int_{\eta_{\varphi_i}^-}^{\eta_{\varphi_i}^+} \psi(\eta, \gamma_i, \underset{\sim}{r}_S) d\eta & \text{if } \eta_\ell^- < \eta_{\varphi_i}^- < \eta_{\varphi_i}^+ < \eta_\ell^+ \quad \text{(F4.2.54d)} \\ = \int_{\eta_\ell^-}^{\eta_{\varphi_i}^+} \psi(\eta, \gamma_i, \underset{\sim}{r}_S) d\eta & \text{if } \eta_{\varphi_i}^- < \eta_\ell^- < \eta_{\varphi_i}^+ < \eta_\ell^+ \quad \text{(F4.2.54e)} \end{cases}$$

Even though at first they may appear somewhat complicated, the limits of integration used for these partial line integrals are obvious when one considers the fact that the global range of integration ($\eta_{\varphi_i}^-, \eta_\ell^+$) may lie totally outside a given eta level (η_ℓ^-, η_ℓ^+), totally inside a given eta level, or overlap the given eta level in any of the ways illustrated in Fig. F4.2.17.

Evaluation of the partial line integrals defined by Eq. (F4.2.54) is rather trivial. Within the bounds of a given eta level (ℓ), the angular flux may be assigned a constant value, $\psi_m(r_S)$, depending on the azimuthal angle γ_i. Ordering the angular fluxes as shown in Fig. F4.2.14, $\psi(\eta, \gamma_i, \underset{\sim}{r}_S)$ may then be written as

$$\psi(\eta, \gamma_i, \underset{\sim}{r}_S) = \psi_m(r_S) , \quad \text{(F4.2.55a)}$$

where

$$\eta_\ell^- < \eta < \eta_\ell^+ \quad \text{(F4.2.55b)}$$

and

$$m = \ell^2 + 2\ell - \text{INT}\left[\frac{\gamma_i}{\left(\frac{\pi}{2\ell}\right)}\right] . \quad \text{(F4.2.55c)}$$

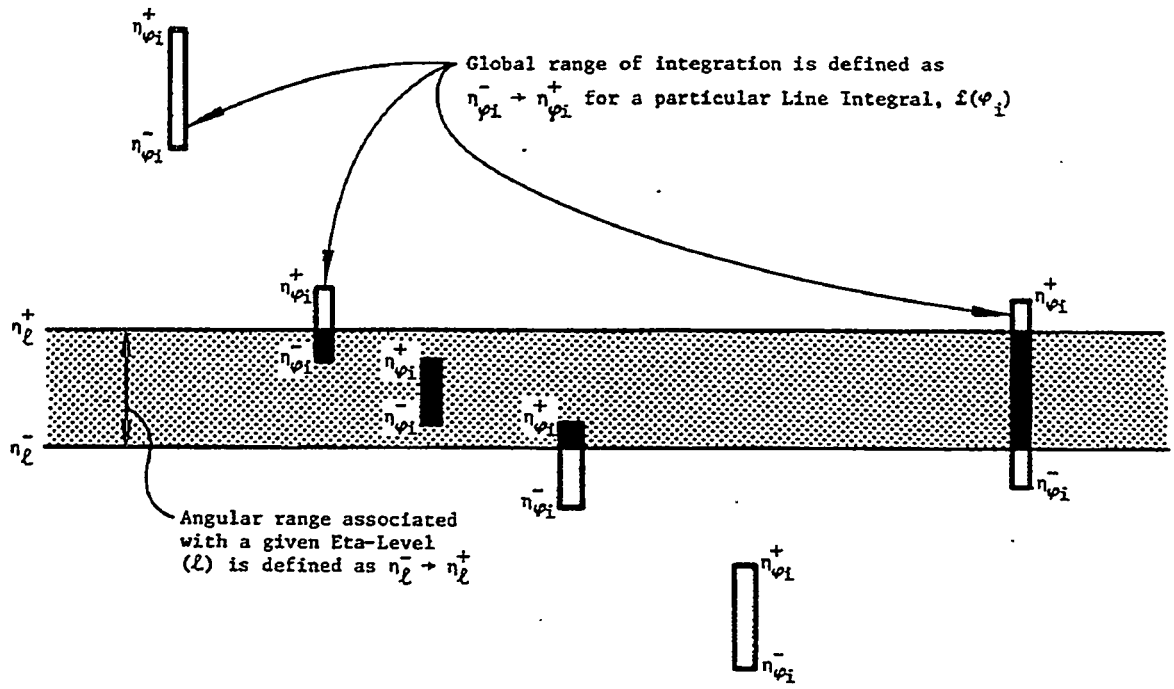


Figure F4.2.17 Various ways in which the global range of integration for a particular line integral [$\mathcal{L}(\varphi_i)$] may overlap the angular range associated with a given eta-level in the angular quadrature

Armed with this information, the partial line integrals defined by Eq. (F4.2.54) may be written explicitly as

$$\mathcal{L}_\ell(\varphi_i) = \begin{cases} = 0 & \text{if } \eta^+_\ell < \eta^-_{\varphi_i} \text{ or } \eta^+_{\varphi_i} < \eta^-_\ell \quad \text{(F4.2.56a)} \\ = (\eta^+_\ell - \eta^-_\ell)\,\psi_m(r_S) & \text{if } \eta^-_{\varphi_i} < \eta^-_\ell < \eta^+_\ell < \eta^+_{\varphi_i} \quad \text{(F4.2.56b)} \\ = (\eta^+_\ell - \eta^-_{\varphi_i})\,\psi_m(r_S) & \text{if } \eta^-_\ell < \eta^-_{\varphi_i} < \eta^+_\ell < \eta^+_{\varphi_i} \quad \text{(F4.2.56c)} \\ = (\eta^+_{\varphi_i} - \eta^-_{\varphi_i})\,\psi_m(r_S) & \text{if } \eta^-_\ell < \eta^-_{\varphi_i} < \eta^+_{\varphi_i} < \eta^+_\ell \quad \text{(F4.2.56d)} \\ = (\eta^+_{\varphi_i} - \eta^-_\ell)\,\psi_m(r_S) & \text{if } \eta^-_{\varphi_i} < \eta^-_\ell < \eta^+_{\varphi_i} < \eta^+_\ell\,, \quad \text{(F4.2.56e)} \end{cases}$$

where m depends on γ_i [as per Eq. (F4.2.55c)] and γ_i depends on φ_i [as per Eq. (F4.2.49)]. Using these results [cf. Eq. (F4.2.56)], and substituting Eq. (F4.2.53b) back into Eq. (F4.2.47), we see that the scalar flux at (r_D, z_D) due to a cylindrical surface source ($r = r_S$, $0 \le z \le h$) located below the detector ($h \le z_D$) is given by

$$\phi_D = 2\left(\frac{\varphi_0}{N}\right) \sum_{i=1}^{N} \sum_{\ell=1}^{L} \mathcal{L}_\ell(\varphi_i)\,, \quad \text{(F4.2.57)}$$

where N is the number of vertical strips the user specifies on the surface of the cylinder between $\varphi = 0$ and $\varphi = \varphi_0$, and L is the number of "eta levels" associated with the given quadrature. Note that the length of the cylinder (h) has no bearing on the number of increments (N) that should be specified, or the calculational time required to evaluate the scalar flux. If the cylindrical surface (h) is not located entirely below the plane of the detector ($z=z_D$), then the scalar flux at the detector may be evaluated by breaking the surface into two component parts (h_1 and h_2), as shown in Fig. F4.2.13. The scalar flux at the detector is then given by

$$\phi_D = \phi_D\Big|_{h_2} + 2\,\phi_D\Big|_{h_1} . \qquad \text{(F4.2.58)}$$

In any event, the calculation is rapid, straightforward, and rather insensitive to the number of increments (N) specified by the user.

[It was stated above the Eq. (F4.2.43) is evaluated numerically by breaking the range of integration ($0 < \varphi < \varphi_0$) into N equal intervals and then summing the partial line integrals [$\pounds_\ell(\varphi_i)$] corresponding to each of the various eta levels. Although that statement is essentially correct, the actual method was programmed slightly differently for reasons that will become clear below. In practice, the order of the summation is reversed and the number of vertical strips in each eta level (N_ℓ) is slightly different, that is,

$$N_\ell = 1 + \mathrm{INT}\left(\frac{\varphi_0}{\Delta\varphi_{i\ell}}\right) , \qquad \text{(F4.2.59a)}$$

where

$$\Delta\varphi_{i\ell} = (\varphi_i^+ - \varphi_i^-) = \left(\frac{\pi}{2\ell}\right) \Big/ (N_{\Delta\varphi}) \qquad \text{(F4.2.59b)}$$

and

$$N_{\Delta\varphi} = 1 + \mathrm{INT}\left[\frac{\left(\frac{\pi}{2\ell}\right)}{\left(\frac{\varphi_0}{N}\right)}\right] . \qquad \text{(F4.2.59c)}$$

In addition, the width of the last vertical strip in each level is compressed so that φ_{last}^+ does not extend beyond φ_0. Note that whenever N is reasonably large ($N \geq 100$), N_ℓ will be almost identical to N. Defined in this fashion, no vertical strip bounded by $(\varphi_i^-, \varphi_i^+)$ will ever "straddle" any of the azimuthal angular ranges $(\varphi_m^-, \varphi_m^+)$ associated with the given quadrature and defined by Eqs. (F4.2.40a-d). The advantage of this, of course, is that as the detector is moved closer and closer to the surface of the cylinder (i.e., as $r_D \rightarrow r_S$, $0 \leq z_D \leq h$), the code is then able to faithfully reproduce the XSDRNPM surface flux even if $N_{\Delta\varphi} = 1$. To be more precise, then, Eq. (F4.2.57) is actually programmed as

$$\phi_D = 2 \sum_{\ell=1}^{L} \left[\Delta\varphi_{i\ell} \sum_{i=1}^{N_\ell} \mathfrak{L}_\ell(\varphi_i) \right] . \qquad \text{(F4.2.60)}$$

As noted above, the method remains extremely fast and rather insensitive to the number of increments (N) specified by the user. Typically, a value of 200 is recommended.

F4.3 FLOWCHART, DESCRIPTION OF SUBROUTINES, AND LIST OF I/O UNITS USED BY XSDOSE

A flow diagram of the XSDOSE code is shown in Fig. F4.3.1. In block form, it shows each of the subroutines and the order in which they are called. A brief description of each routine is provided below. [Parenthetically, we note that the SCALE version of XSDOSE has two main programs – one having an unnamed entry point (MAIN), which is accessed when the SCALE driver sees =XSDOSE in the input stream, and an alias entry point routine (Q#$102), which is accessed when the SCALE driver sees =Q#$102 in the input stream as entered by the user or one of the control modules (SAS1, SAS2, etc.). In the first case (=XSDOSE), the code will read card-image input data supplied on logical unit 5; in the second case (=Q#$102), the code expects the input to be supplied in binary format on logical unit 95. Each of the main entry point routines is ~14 cards long. In the one case, a variable called BINPUT is initialized to 0, whereas in the second case it is initialized to 95. That is the only difference between the two.] A more detailed description of the various subroutines now follows:

MAIN (unnamed entry point) – opens buffer space for various I/O units and then calls ALOCAT which, in turn, calls DOSER; initializes binary input flag to "no."

MAIN (Q#$102) – opens buffer space for various I/O units and then calls ALOCAT which, in turn, calls DOSER; initializes binary input flag to "yes."

ALOCAT – an Assembly language routine from the SCALE Subroutine Library; it determines the amount of core storage available in the system and allocates it for use in subroutine DOSER (i.e., it sets the size limit for the large container array [D] used by DOSER).

DOSER – functionally this acts as the main routine for XSDOSE; it calls AREAD, IREAD, and FREAD to read the card-image input, or, alternatively, it reads the binary input on logical unit 95; it calls subroutine DOQ to reconstruct the quadrature set (i.e., the direction cosines and quadrature weights) used in the previous XSDRNPM calculation; it calls subroutine BAND to establish the angular ranges or "boundaries" associated with the given quadrature set; it calls DFACTR to read the flux-to-dose conversion factors off the cross-section library on unit N86; it calls PRNTID to print a list of all dose factor IDs input by the user; it edits the quadrature set calculated by DOQ; it reads the angular flux file made by XSDRNPM and temporarily stored on unit N16; it then edits the angular fluxes; it calls subroutine FCALC to calculate the multigroup scalar flux at each detector site; it calls REDUCE to compress the double-precision scalar fluxes calculated by FCALC down to single-precision variables; and lastly, at each detector site, it (a) calls SFLUX to edit the multigroup scalar fluxes, (b) calls DDOSE to calculate the edit the neutron doses corresponding to each set of neutron dose factors, and (c) calls DDOSE to calculate and edit the gamma doses corresponding to each set of gamma dose factors.

AREAD, IREAD, FREAD – FORTRAN routines from the SCALE Subroutine Library which are used to read alphanumeric, integer, and floating-point input data in a "free-form" format.

DOQ – given the type of geometry (IGE = 1/2/3, slab/cylindrical/spherical) and the order of the quadrature (ISN), this routine calculates the direction cosines and quadrature weights used by XSDRNPM and XSDOSE; for a mathematical description of the various types of quadrature sets generated, see Sect. C1.3.6.

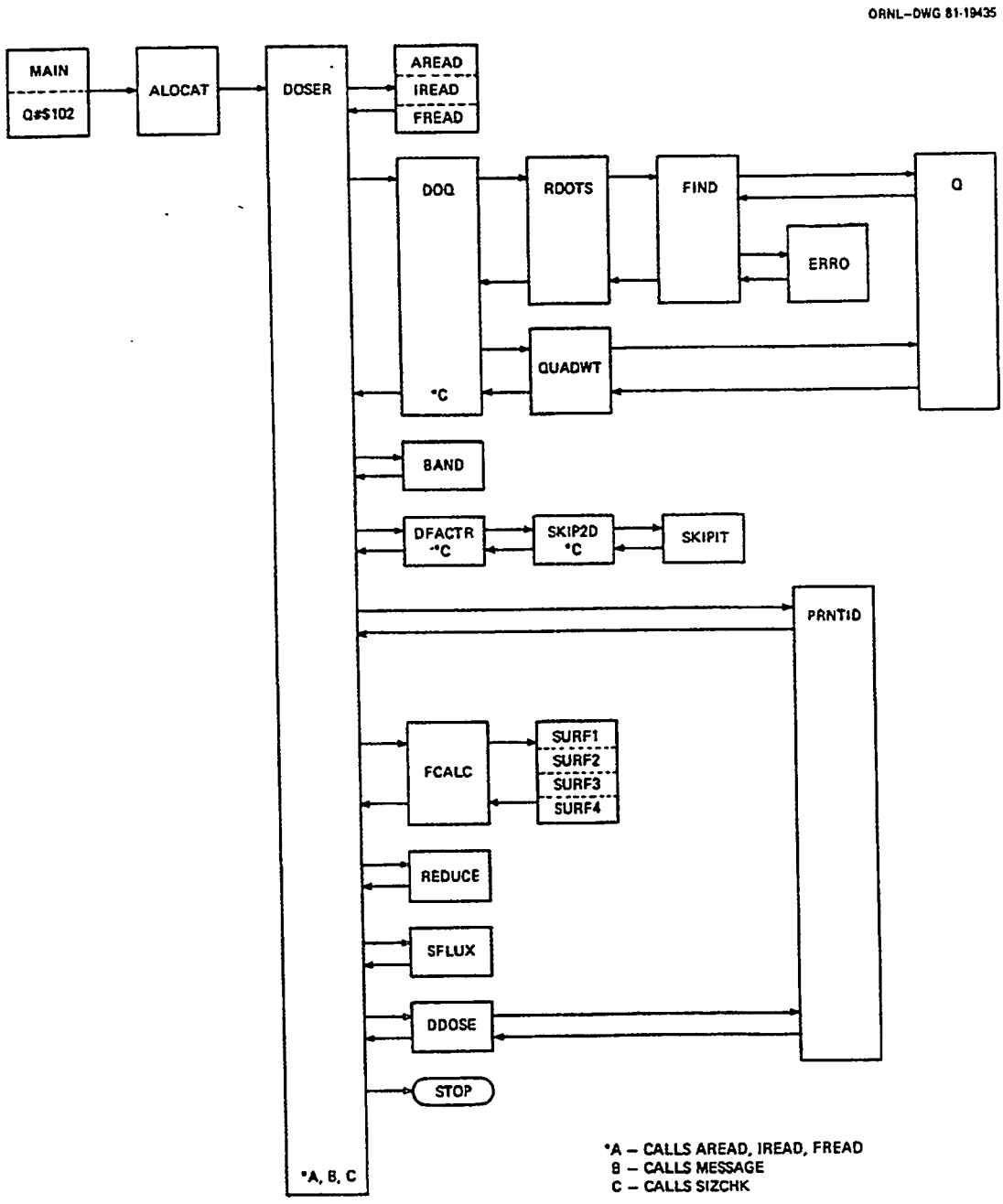


Figure F4.3.1 Flowchart showing all the subroutines used by XSDOSE and the order in which they are called

ROOTS – finds the (n/2) positive roots of $P_n(x) = 0$, where n = ISN/2 for slab geometry, or n = (ISN+1)/2 for cylindrical and spherical geometry; first it finds the roots of $P_2(x) = 0$, then $P_3(x) = 0$, then $P_4(x) = 0$, etc.; it takes advantage of the fact that the roots of successive Legendre polynomials are interleaved.

FIND – given the (n-1)/2 negative roots of $P_{n-1}(x) = 0$, this routine calculates the (n/2) negative roots of $P_n(x) = 0$; it takes advantage of the fact that the roots of successive Legendre polynomials are interleaved, and applies a "binary split" search procedure to find each new root.

Q – given n and x, this routine evaluates the Legendre polynomial $P_n(x)$, and returns the calculated value as $Q(n,x) = P_n(x)$.

ERRO – prints a one-line error message if, in subroutine FIND, subroutine Q returns a value of $P_n(x)$ having the wrong sign; in practice, this routine is never called.

QUADWT – given the (n/2) positive roots of $P_n(x) = 0$, this routine calculates the corresponding Gaussian quadrature weights and returns with $\{x_i, w_i; i = 1, \ldots, n\}$.

BAND – given a unit sphere over all solid angle (cf. Fig. F4.2.3 or Fig. F4.2.12), this subroutine calculates the boundaries (μ_m^-, μ_m^+) associated with a given quadrature set $\{\mu_i, w_i\}$ in spherical or slab geometry, or the boundaries (η_ℓ^-, n_ℓ^+) associated with the various eta-levels of a given quadrature $\{\eta_i, \mu_i, w_i\}$ in cylindrical geometry.

DFACTR – reads the multigroup neutron and/or gamma-ray flux-to-dose conversion factors off the AMPX Master or Working cross-section library found on logical unit N86; number of neutron groups (NG) and number of gamma groups (I1) are also read off this file; calls SKIP2D if this is an AMPX Master library, but does not call SKIP2D if this is an AMPX Working library; for details regarding the exact format of these two types of cross-section libraries, see Sect. 11.3.5 and/or Sect. 11.4 of the AMPX User's Guide, ORNL/TM-3706 (March 1976).

SKIP2D – this routine sets up the pointers which enable SKIPIT to read "over" those reactors containing the cross-section data for the (2-D) group-to-group transfer arrays.

SKIPIT – reads over those records containing the (2-D) group-to-group Legendre transfer coefficients for a given (n,n), (n,γ) or (γ,γ) process. [For (n,γ) or (γ,γ) processes it will read one record containing all the P_0 group-to-group transfer coefficients, another for the P_1 coefficients, etc., until it has read the $(N+1)^{st}$ record containing the P_N coefficients. This (n,γ) and (γ,γ) data are temperature-independent. The (n,n) data, however, is temperature-dependent. Thus, for (n,n) data, it first reads over a record containing a list of temperatures at which data are available; for the first temperature it then reads over one record containing the P_0 group-to-group transfer coefficients, another for the P_1 coefficients, etc., until it has read the $(N+1)^{st}$ record containing the P_N coefficients; this process in then repeated for each of the temperatures at which data are available.]

PRNTID – for every dose factor ID number it is given, this routine prints a single descriptive line of output giving the name of the dose factor data set (ANSI-Standard, Straker-Morrison, etc.) and the associated units (Rem/hr, etc.); it recognizes only those IDs listed in Table F4.4.1.

FCALC – depending upon the geometry (IGE), this routine will call SURF1, SURF2, SURF3, or SURF4 to calculate the multigroup scalar flux at each detector location.

SURF1 – calculates the multigroup scalar flux at a point some distance from a rectangular surface source.

SURF2 – calculates the multigroup scalar flux at a point some distance from the side of a finite cylindrical source.

SURF3 – calculates the multigroup scalar flux at a point some distance from a spherical surface source.

SURF4 – calculates the multigroup scalar flux at a point some distance from a circular, disc-shaped source.

REDUCE – takes the double-precision multigroup scalar fluxes calculated by FCALC and stored in the D array, converts them to single precision, and compresses out the "extra space" left in the D array (i.e., it extracts the odd elements of an array and redefines them as $a_i = a_{2i-1}$, i = 1, ..., N).

SFLUX – prints an edit of the multigroup neutron (scalar) flux and the multigroup gamma (scalar) flux at a given detector.

DDOSE – given the multigroup scalar fluxes (for either the neutron or the gamma energy groups) at a given detector site, this routine prints an edit of those multigroup scalar fluxes, the corresponding flux-to-dose conversion factors, the calculated dose due to each energy group, and the total neutron (or gamma) dose at that particular detector site.

SIZCHK – small utility routine that determines whether there is adequate space left in core to append a new array onto the end of the large, flexibly dimensioned D array; prints error message and corrective action to be taken if space left is insufficient; called by DOSER, DOQ, DFACTR, and SKIP2D.

Other Routines From the SCALE Subroutine Library That are Used by XSDOSE:

AREAD, IREAD, FREAD – FORTRAN routines used by DOSER to read alphanumeric, integer, and floating-point input data in a "free-form" format.

MESAGE – used by DOSER to print header pages with big block letters; calls DATIM and FHLPR.

DATIM – machine language program to determine the date and time.

FHLPR – prints eight "block letter" characters across a page.

ALOCAT – an Assembly Language routine; it determines the amount of core storage available in the system and allocates it for use in subroutine DOSER (i.e., it sets the size limit for the large container array [D] used by DOSER).

Input/Output Units Used by XSDOSE:

Logical Unit	Purpose
5	Card input
6	Printed output
16	Dummy file that is opened so as to reserve buffer space for N16 before calling ALOCAT
86	Dummy file that is opened so as to reserve buffer space for N86 before calling ALOCAT
N16	Angular fluxes from XSDRNPM; User defines N16; Usually N16 = 16
N86	Cross-section library containing dose factors; User defines N86; Often N86 = 86

F4.4 INPUT INSTRUCTIONS FOR XSDOSE

XSDOSE is typically used in conjunction with a fixed-source XSDRNPM calculation for an infinite slab, cylinder, or sphere. XSDOSE then reads the angular flux file produced by XSDRNPM and performs the required numerical integration over a finite surface to obtain the actual scalar flux at those points specified by the user.

For convenience, XSDOSE reads the angular flux file produced by XSDRNPM and extracts the information it needs. To be more specific, XSDRNPM saves the (REAL*8) angular fluxes on logical unit N16. For each energy group, there is a single binary record written in the following format:

$$((\psi(i,n), i = 1, IM + 1), n = 1,MM) , \qquad \text{(F4.4.1)}$$

where IM is the number of spatial intervals, and MM [= (ISN+1) or ISN*(ISN + 4)/4] is the number of discrete angles used in the XSDRNPM calculation. XSDOSE reads this binary file and saves only the angular fluxes on the right-hand boundary:

$$(\psi(i = IM + 1, n), n = 1,MM) . \qquad \text{(F4.4.2)}$$

This angular flux distribution, which is assumed to be independent of position, is then used in the numerical integration over the finite surface shown in Fig. F4.4.1.

To calculate the flux and/or dose at a point some distance from the end of a cylinder ($r_D \leq$ DIMEN1), one may perform a 1-D XSDRNPM calculation in slab geometry along the axis of the cylinder, and set IGE=4 in the corresponding XSDOSE calculation. The angular flux distribution on the right-hand boundary of the XSDRNPM model will then be used in the numerical integration over the circular disc shown in Fig. F4.4.1d.

To estimate the total flux and/or dose at points above but "off to the side" of a finite cylinder ($r_D >$ DIMEN1, $z_D >$ DIMEN2), one could combine the results of two XSDRNPM/XSDOSE calculations – one with IGE = 2 and one with IGE = 4.

Many shielding calculations require the user to compute the flux and other energy-dependent response functions at various points of interest. For convenience, XSDOSE is designed to read any number of multigroup response functions off an AMPX master library or an AMPX working library [cf. Sects. 11.3.5, 11.4, and 11.5 of the AMPX User's Guide, ORNL/TM-3706 (March 1976)]. This library may be a neutron cross-section library, a gamma cross-section library, or a fully coupled n-γ library. Even though the cross-section library used by XSDOSE may or may not be the same as that used in the XSDRNPM calculation, the energy group structure must at least be the same. The other thing to note is that XSDOSE expects to find nuclide #500000 in the cross-section library. This fictitious Nuclide ID number identifies a collection of multigroup response functions. Each multigroup response function is then individual identified by a material-process number (i.e., an MT number). Although the data associated with a given MT number may generally represent a set of flux-to-dose conversion factors, a material damage function, or some detector response function, those numbers listed in Table F4.4.1 have been reserved for specific sets of flux-to-dose conversion factors.

The free-form input processor implemented in XSDOSE allows both integer and floating-point data to be entered in an unformatted manner. All 80 columns of any card may be used, and data can start or end in any column. Any data entry must, however, be followed by one or more blanks. Integers may be used for floating values if the particular item has no decimal value (i.e., 10 will be interpreted as 10.0). Likewise, 1+4, 1.0+4, 1.0E+4, or 10000.0 will all be interpreted as 1.0×10^4. Note that imbedded blanks are not allowed within the representation for a given number. The only exception to this is that a single blank may

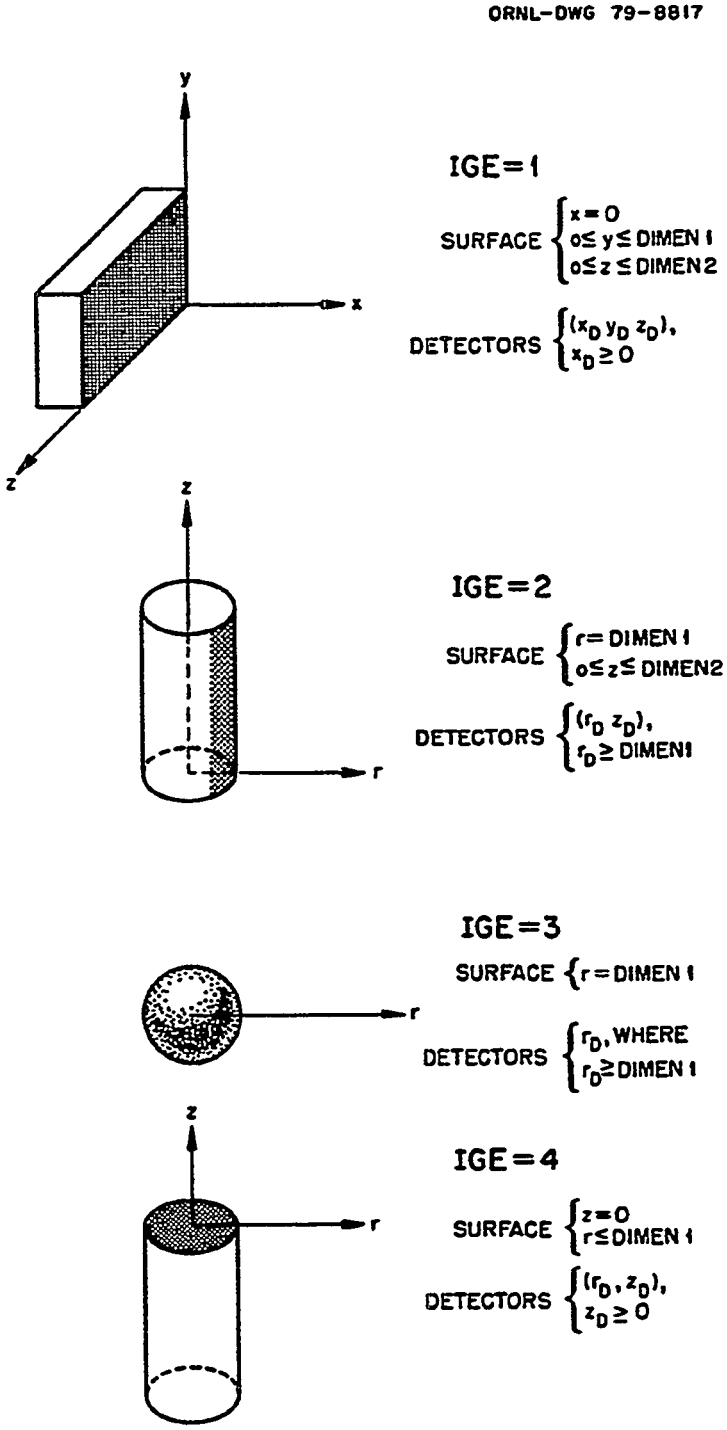


Figure F4.4.1 Geometry options available in XSDOSE

Table F4.4.1. Special dose factor ID numbers that have been reserved for specific response functions

MT No.	Response Function
9001	Hurst dose factors (mrad/h)/(n/cm^2/s)
9002	Snyder-Neufeld dose factors (mrad/h)/(n/cm^2/s)
9026	Snyder-Neufeld conversion from flux to biological dose (mrem/h)/(n/cm^2/s)
9027	Henderson conversion from neutron flux to absorbed dose rate in tissue (rad/h)/(n/cm^2/s)
9028	Straker-Morrison conversion factors (mrem/h)/(n/cm^2/s)
9029	ANSI standard neutron flux-to-dose-rate factors (rem/h)/(n/cm^2/s)
9501	Straker-Morrison conversion factors (mr/h)/(gamma-ray/cm^2/s)
9502	Henderson conversion factors (rad/h)/(photons/cm^2/s)
9503	Claiborne-Trubey conversion factors (rad/h)/(photons/cm^2/s)
9504	ANSI standard gamma-ray flux-to-dose-rate factors (rem/h)/(photons/cm^2/s)

precede an unsigned exponent in a floating-point number. Thus, for example, 1.0E 04 would be correctly interpreted as 1.0×10^4. Note that imbedded blanks are not allowed within the representation for a given number. The only exception to this is that a single blank may precede an unsigned exponent in a floating-point number. Thus, for example, 1.0E 04 would be correctly interpreted as 1.0×10^4.

This free-form processor has provisions for multiple entries of the same data value. This step is accomplished by entering the number of repeats, followed by either R, *, or $, followed by the data value to be repeated. For example, 5R2 or 5*2 enters five successive 2's in the input data. There should be no blanks between the number of repeats and the repeat flag (R; *, or $), but each multiple entry must be separated from the rest of the data by one or more blanks. Multiple zeros may be specified as nZ, where n is the number of zeros to be repeated. There should not be any blanks between the n and the Z, but the nZ must be separated from the rest of the data by one or more blanks.

****

The actual input for XSDOSE has been divided into six blocks:

1. THE MODULE SPECIFICATION CARD
2. THE TITLE CARD
3. THE PARAMETER CARD
4. DOSE FACTOR ID NUMBERS
5. COORDINATES FOR DETECTOR POINTS
6. THE END CARD

As many data cards as necessary may be used to describe any given data block, but each block must begin on a new data card. Each of these blocks will now be described in detail:

1. THE MODULE SPECIFICATION CARD

The seven characters =XSDOSE must be punched in columns 1 through 7.

2. THE TITLE CARD

All 80 columns may be used for a descriptive title.

3. THE PARAMETER CARD (11 entries required)

1. IGE — Source distribution (see Fig. F4.4.1)
   Enter 1 for a rectangular surface source
   Enter 2 for a cylindrical surface source
   Enter 3 for a spherical surface source
   Enter 4 for a flat, circular, disc-shaped source
2. IM — Number of mesh intervals used in the previous XSDRNPM calculation.
3. ISN — Order of quadrature used in the previous XSDRNPM calculation. (XSDOSE will use the same algorithms found in XSDRNPM to reconstruct the angular directions and quadrature weights used in the previous calculation.)
4. N16 — Logical unit on which angular fluxes are to be read. (Normally, XSDRNPM will write the angular fluxes on logical unit 16.)
5. N86 — Logical unit for the cross-section library containing the flux-to-dose conversion factors. See note above.
6. MAST — Enter 1 if the cross-section library containing the flux-to-dose conversion factors is an AMPX master library.
   Enter 0 if the cross-section library containing the flux-to-dose conversion factors is an AMPX working library.
7. NDETEC — Number of detectors (i.e., number of points at which the dose is to be calculated). Coordinates for these detectors will be entered in Block 5 below.
8. NFACTR — Number of Dose Factor ID numbers the user intends to enter in Block 4 below.
9. NINCRM — Number of increments used in the numerical integration. Even though any number of increments may be used, five- or six-digit accuracy is usually obtained using 200 increments. Such a calculation typically takes less than one second per detector on the IBM-360/91. Unlike previous codes, the number of increments required for this type of accuracy is independent of the location of the detector(s).
10. DIMEN1 — Primary dimension (cm) describing the extent and/or location of the surface source. See Fig. F4.4.1;
    If IGE = 1 / 2 / 3 / 4 , then
    DIMEN1 = y_{max} / r_{cyl} / r_{sph} / r_{disc} .
11. DIMEN2 — Auxiliary dimension (cm) describing the extent and/or location of the surface source.
    If IGE = 1 or 2, DIMEN2 = z_{max} (cf. Fig. F4.4.1);
    If IGE = 3 or 4, enter zero.

4. DOSE FACTOR ID NUMBERS

Any number of Dose Factor IDs may be entered. Many of the commonly used ones are listed in TableF4.4.1. To compute the ANSI-Standard neutron dose and the ANSI-Standard gamma dose at each detector, one would, for example, enter 9029 and 9504. At least one entry is required in this data block. If a particular set of flux-to-dose conversion factors is not available on the given cross-section library, XSDOSE will simply skip that particular edit and continue.

As noted above, one may also use XSDOSE to calculate the response of a flux detector or the radiation damage inflicted upon a certain material, by entering the appropriate MT number(s) in this data block. If a

particular response function is not available on the cross-section library, XSDOSE will simply skip that particular edit and continue.

As noted above, one may also use XSDOSE to calculate the response of a flux detector or the radiation damage inflicted upon a certain material, by entering the appropriate MT number(s) in this data block. If a particular response function is not available on the cross-section library, XSDOSE will simply skip that particular edit and continue.

5. COORDINATES FOR DETECTOR POINTS (See Fig. F4.4.1)

If IGE = 1, enter $x_{D1}\ y_{D1}\ z_{D1}\ \ x_{D2}\ y_{D2}\ z_{D2}\ \ x_{D3}\ y_{D3}\ z_{D3}$, etc.

If IGE = 2, enter $r_{D1}\ z_{D1}\ \ r_{D2}\ z_{D2}\ \ r_{D3}\ z_{D3}$, etc.

If IGE = 3, enter $r_{D1}\ r_{D2}\ r_{D3}$, etc.

If IGE = 4, enter $r_{D1}\ z_{D1}\ \ r_{D2}\ z_{D2}\ \ r_{D3}\ z_{D3}$, etc.

The location of the detector coordinates relative to the various surfaces is illustrated in Fig. F4.4.1. All dimensions are in centimeters.

6. THE END CARD

The user should enter a final card with END punched in columns 1 through 3.

NOTE: Because of the limited amount of input required by the XSDOSE code, it does not have any "built-in" error messages. "End of file on unit 5" is about the only error that ever occurs. If that should occur: (1) make sure the END card was included, with END punched in columns 1 through 3; (2) make sure that the number of detector coordinates entered in Block 5 corresponds to the number of detectors specified by NDETEC; and (3) make sure that the number of Dose Factor ID's entered in Block 4 corresponds to that specified by NFACTR. Frequently people will take an input deck that works and then add or delete data from one of the data blocks while forgetting to make the corresponding change on the Parameter Card. This error is probably the most common type of input error.

F4.5 SAMPLE PROBLEM

The purpose of XSDOSE is to calculate the scalar flux and corresponding dose rate at points some distance from a finite 1-D surface on which the angular flux distribution is known. Typically, the angular flux on the surface of the body is calculated using a 1-D transport code such as XSDRNPM. To illustrate how the two codes may be used together, consider the situation depicted in Fig. F4.5.1. There we have a large rail cask measuring ~2m in diameter by ~5m long. At the midplane of the cask (Z = 254 cm) we wish to determine the dose at the surface, 3 ft (91.44 cm) from the surface, and 10 ft (308.4 cm) from the centerline. We would also like to calculate the dose near the end of the cask, 10 ft from the centerline (Z = 508 cm, r = 308.4 cm). So that the example is as realistic and as useful as possible, we have included below:

(1) a physical description of the cask,
(2) a listing of the XSDRNPM input (along with a brief explanation of that input),
(3) a listing of the XSDOSE input (along with a brief explanation of that input),
(4) an abbreviated listing of the XSDRNPM output, and
(5) a complete listing of the XSDOSE output.

Because the XSDOSE code always requires an angular flux file as input, we deemed it necessary to include some details of the XSDRNPM input along with the present example. So that the input for both codes would be "complete" in the context of the SCALE system, we have used the DLC-23 22-neutron-group 18-gamma-group working cross-section library, which is available as part of the SCALE system on logical unit number 85.*

F4.5.1 DETAILED PHYSICAL DESCRIPTION OF THE PROBLEM

The location of the detector points relative to the cask are shown in Fig. F4.5.1. Note that the cask is 198.01 cm in diameter and extends from Z = 0 to Z = 508 cm. (In the XSDRNPM calculation, the cask will be treated as an infinite cylinder with no buckling correction.) The cask itself is shown in Fig. F4.5.2. It consists of an inner steel shell, a Pb gamma shield, an outer steel shell, a neutron shield, and an outside barrel. The three steel components are assumed to be SS-304 (69.5 wt % Fe, 19 wt % Cr, 9.5 wt % Ni, and 2 wt % Mn). By volume, the neutron shield consists of 28.5% water (1.0 g/cc), 66.0% ethylene glycol ($HOCH_2CH_2OH$ at 1.11 g/cc), and 5.5% potassium tetraborate ($K_2B_4O_7*8H_2O$ at 1.74 g/cc). By weight, this common mixture of water and antifreeze contains ~1% natural boron.

The interior of the cask (which we will represent as a single homogenized region) contains a large monolithic aluminum cylinder (cf. Fig. F4.5.3) having 15 square holes, each measuring 22.1 cm x 22.1 cm, and each containing a dry PWR spent fuel assembly. Each 15 × 15 assembly has 21 pins removed, leaving a total of 204 Zircaloy-clad fuel pins per assembly. The spent fuel consists of 10.33 g/cc UO_2 (0.84 wt % ^{235}U and 99.16 wt % ^{238}U) and 0.077 g/cc PuO_2 (70.77 wt % ^{239}Pu and 29.23 wt % ^{240}Pu). The fuel pins are

*At the time that this sample problem was formulated, the 22n-18γ cross-section library referred to here was available in the SCALE system in the form of an AMPX "working" library. Since that time, the data has been recast into the form of an AMPX "master" library. To convert the data from the master library format into the working library format required by XSDRNPM would now require an additional NITAWL step, as described in the footnote to Table F4.5.3.

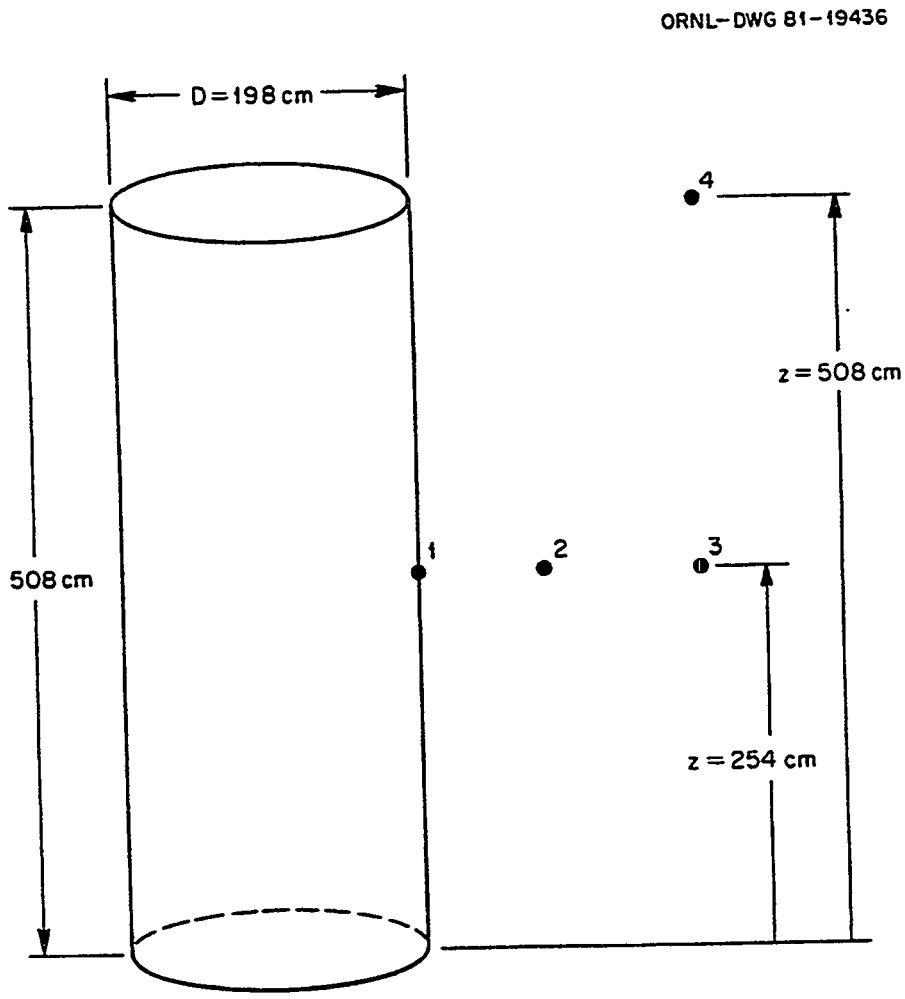


Figure F4.5.1 Location of detectors 1, 2, 3, and 4 relative to the surface of a large spent fuel shipping cask ($R_1 = R_S = 99.005$ cm, $R_2 = R_S + 91.44$ cm $= 190.445$ cm, $R_3 = R_4 = 304.8$ cm)

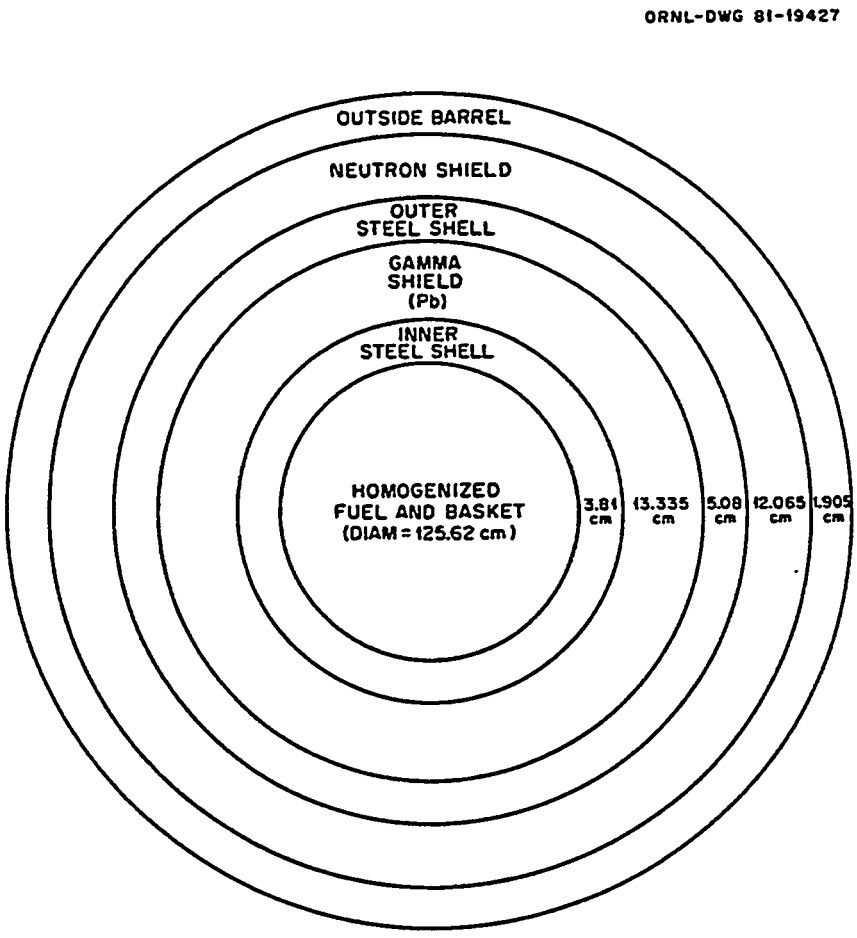


Figure F4.5.2 One-dimensional radial model of the spent fuel shipping cask used in the XSDRNPM shielding calculation

spaced on a 1.430-cm pitch and are 1.072 cm in diameter. The fuel pellets are 0.929 cm in diameter, and the Zircaloy clad is 0.0617 cm thick. Homogenized number densities for the region are given in Table F4.5.1.

The neutron/gamma source strength in the homogenized fuel/basket region depends on the number of spent fuel assemblies (15) and the age of the spent fuel. For the 2-year-old spent fuel considered in this example, ORIGEN-2 calculations have shown the fuel to generate 1.098×10^{8} (n/s)/assembly and 2.147×10^{16} (p/s)/assembly. The neutron/gamma spectra for this 2-year-old PWR fuel is shown in Table F4.5.2. For the purpose of normalizing the source strength in the XSDRNPM calculation, assume that the active length of the fuel is 365.76 cm.

F4.5.2 BRIEF EXPLANATION OF THE XSDRNPM INPUT FOR THIS SAMPLE PROBLEM

The input data for this particular sample problem are shown in Table F4.5.3. A detailed description of the XSDRNPM input requirements is, of course, given in Sect. F3. For completeness, we include here a brief explanation of the input required for this particular problem:

0$$ Array – Used to tell the code that the cross-section library to be used is found on logical unit 85.

1$$ Array – The 15 parameters shown here specify (1) cylindrical geometry, (2) 6 zones, (3) 100 mesh intervals, (4) reflected boundary condition at the centerline, (5) vacuum boundary condition on the surface, (6) 4 mixtures, (7) 18 entries in the mixing table (cf. Table F4.5.1), (8) S_{12} quadrature, (9) P_3 scattering, (10) fixed-source calculation, (11) up to 100 inner iterations allowed per outer (12) up to 20 outer iterations allowed, (13) always use S_n theory, (14) forward calculation, (15) use weighted diamond-difference model exclusively.

3$$ Array – Tells code that a volumetric source spectra will be supplied later (cf. the 31** Array shown below).

5** Array – Source normalization factor (XNF) is set as follows:

$$\text{XNF} = \left(\begin{matrix}\text{No. of}\\ \text{assemblies}\end{matrix}\right)\left[\left(\frac{\text{n/s}}{\text{assembly}}\right) + \left(\frac{\text{photons/s}}{\text{assembly}}\right)\right] \Big/ \left(\begin{matrix}\text{active length}\\ \text{of the fuel}\end{matrix}\right)$$

$$\text{XNF} = (15)\,[(1.098 \times 10^{8}) + (2.147 \times 10^{16})]/(365.76\ \text{cm})$$

$$\text{XNF} = 8.805 \times 10^{14}$$

13$$ Array – Mixture number corresponding to each entry in the mixing table (cf. Table F4.5.1).

14$$ Array – Nuclide ID number corresponding to each entry in the mixing table (cf. Table F4.5.1).

15** Array – Number density (atoms/b-cm) corresponding to each entry in the mixing table (cf. Table F4.5.1).

30$$ Array – Says that "volumetric source spectra number 1" will be used in each of the first 24 mesh intervals and that no source will be used anywhere else; the location of these mesh intervals will be supplied below, in the 35** array.

31** Array – Specifications for "volumetric source spectra number 1." Because this is a 40-group calculation, there will be 40 entries in this array. The first 22 entries will correspond to the neutron spectra of Table F4.5.2a, multiplied by the neutron source per assembly:

$\chi_1 = 1.098(+8) \times 1.186(-4) = 1.302(+4)$

$\chi_2 = 1.098(+8) \times 1.008(-3) = 1.107(+5)$

$\chi_3 = 1.098(+8) \times 2.772(-3) = 3.044(+5)$

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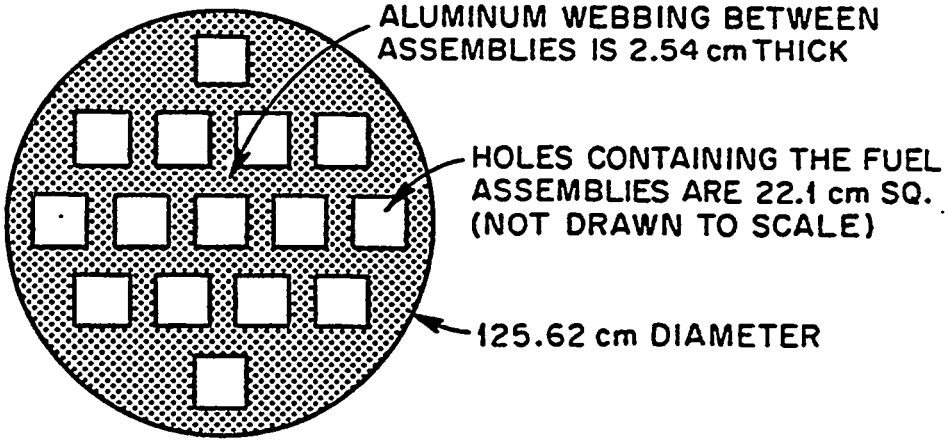


Figure F4.5.3 Removable aluminum basket used to hold 15 PWR fuel assemblies in the center region of the cask

Table F4.5.1 Composition of materials used in the shipping cask problem

Mixture	Mixture No.	Nuclide	Nuclide ID No.	No. density atoms/(b-cm)
Fuel/basket	1	^{235}U	92235	3.11(-5)
Fuel/basket	1	^{238}U	92238	3.65(-3)
Fuel/basket	1	^{239}Pu	94239	1.94(-5)
Fuel/basket	1	^{240}Pu	94240	8.84(-6)
Fuel/basket	1	O	8016	7.41(-3)
Fuel/basket	1	Zr	40000	2.12(-3)
Fuel/basket	1	Al	13027	2.46(-2)
SS-304	2	Fe	26000	5.94(-2)
SS-304	2	Cr	24000	1.74(-2)
SS-304	2	Ni	28000	7.72(-3)
SS-304	2	Mn	25055	1.74(-3)
Gamma shield	3	Pb	82000	3.30(-2)
Neutron shield	4	H	1001	6.41(-2)
Neutron shield	4	C	6012	1.42(-2)
Neutron shield	4	O	8016	2.60(-2)
Neutron shield	4	^{10}B	5010	1.15(-4)
Neutron shield	4	^{11}B	5011	4.96(-4)
Neutron shield	4	K	19039	3.05(-4)

Table F4.5.2 Neutron/gamma spectra for the 2-year-old PWR spent fuel (to be used with the DLC-23 22n-18γ cross-section library)

Neutron group	Spectra	Gamma group	Spectra
1	1.186E-04	1	2.643E-12
2	1.008E-03	2	1.725E-11
3	2.772E-03	3	1.055E-10
4	1.384E-02	4	9.978E-11
5	3.497E-02	5	3.287E-06
6	4.934E-02	6	2.630E-05
7	1.388E-01	7	1.456E-03
8	1.108E-01	8	6.167E-04
9	2.582E-02	9	7.705E-03
10	1.280E-01	10	1.439E-02
11	2.171E-01	11	4.420E-02
12	1.899E-01	12	1.068E-01
13	8.750E-02	13	1.346E-01
14	4.305E-06	14	1.491E-02
15	0.0	15	2.693E-02
16	0.0	16	6.407E-02
17	0.0	17	9.981E-02
18	0.0	18	4.845E-01
19	0.0		
20	0.0		1.000E+00
21	0.0		
22	0.0		
	1.000E+00		

Table F4.5.3. Sample problem input for XSDRNPM and XSDOSE*

```
=XSDRNPM
PB CASK CONTAINING 15 2-YEAR-OLD PWR FUEL ASSEMBLIES
0$$ A3 85 E    1$$ 2 6 100 1 0 4 18 12 3 0 100 20 0 0 3
3$$ A2 1 E     5** A3 8.805+14 E    T
13$$  7R1 4R2 3 6R4
14$$ 92235 92238 94239 94240 8016 40000 13027 26000 24000
     28000 25055 82000 1001 6012 8016 5010 5011 19000
15** 3.11-5 3.65-3 1.94-5 8.84-6 7.41-3 2.12-3 2.46-2 5.94-2 1.74-2
     7.72-3 1.74-3 3.30-2 6.41-2 1.42-2 2.60-2 1.15-4 4.96-4 3.05-4    T
30$$ 24R1 F0
31** 1.302+4 1.107+5 3.044+5 1.520+6 3.840+6 5.418+6 1.524+7 1.217+7
     2.835+6 1.405+7 2.384+7 2.085+7 9.608+6 4.727+2 8Z
     5.675+4 3.704+5 2.265+6 2.142+6 7.057+10 5.647+11 3.126+13
     1.324+13 1.654+14 3.090+14 9.490+14 2.293+15 2.890+15 3.201+14
     5.782+14 1.376+15 2.143+15 1.040+16    T
33** F0     T
35** 23I0 6I62.81 41I66.62 7I79.955 14I85.035 3I97.1 99.005
36$$ 24R1 7R2 42R3 8R4 15R5 4R6    39$$ 1 2 3 2 4 2    40$$ F3    T
END
=XSDOSE
PB CASK CONTAINING 15 2-YEAR-OLD PWR FUEL ASSEMBLIES
2  100  12  16  85  0  4  2  200  99.005  508.0
9028  9501
99.005  254    190.445  254    304.8  254    304.8  508
END
//
```

*At the time that this sample problem was executed, the SCALE 22n-18γ cross-section library on logical unit 85 was in the form of an AMPX "working" library. Since that time, the data have been recast into the form of an AMPX "master" library. To convert the data from the master library format to the working library format required by XSDRNPM, the user should now include the following NITAWL data immediately before the XSDRNPM data:

```
=NITAWL
0$$  85  E    1$$  F0  A2  18  E    T
2$$ 92235 92238 94239 94240 40000 13027 26000 24000
28000 25055 82000 1001 6012 8016 5010 5011 19000 500000     T
```

A detailed description of the NITAWL input may be found in Sect. F2. In this case, the "extra" NITAWL step simply copies the data for these nuclides from the master library on logical unit 85 to a working library on logical unit 4. In the corresponding XSDRNPM calculation, the data for the 0$$ Array (0$$ A3 85 E) should be deleted, or the "85" should be changed to a "4." Likewise, the "85" on the XSDOSE parameter card should be changed to a "4," or the "0" should be changed to a "1."

while the last 18 entries will correspond to the photon spectra of Table F4.5.2b, multiplied by the total photon source per assembly:

$\chi_{23} = 2.147(+16) \times 2.643(-12) = 5.675(+4)$
$\chi_{24} = 2.147(+16) \times 1.725(-11) = 3.704(+5)$
$\chi_{25} = 2.147(+16) \times 1.055(-10) = 2.265(+6)$

Note that 8Z was used to denote the last eight entries in the neutron spectra where χ_i was zero. Also note that the spectrum need not sum to 1.0 when specified in this fashion.

33** Array – Defaults the initial flux guess to 0.0 everywhere.

35** Array – Specifies the mesh boundaries; must have 101 entries since we earlier specified that we had 100 mesh intervals; interpreted in the following fashion: (1) we have one mesh boundary at R=0.0 cm, 62.81 cm, 66.62 cm, 79.955 cm, 85.035 cm, 97.1 cm, and 99.005 cm; (2) between 0.0 and 62.81 cm, we have 23 other mesh boundaries uniformly spaced; (3) between 62.81 cm and 66.62 cm, we have six other mesh boundaries uniformly spaced; etc.

36$$ Array – Says the first 24 mesh intervals are in zone 1, the next 7 are in zone 2, the next 42 are in zone 3, etc.

39$$ Array – Mixtures 1, 2, 3, 2, 4, and 2 are to be assigned to zones 1, 2, 3, 4, 5, and 6, respectively.

40$$ Array – Tells code to use P_3 scattering in each zone.

F4.5.3 BRIEF EXPLANATION OF THE XSDOSE INPUT FOR THIS SAMPLE PROBLEM

The input data for this particular sample problem are shown in Table F4.5.3. A detailed description of the XSDOSE input requirements is, of course, given in Sect. F4.4. For completeness, we include here a brief explanation of the input required for this particular problem:

First Card – Title Card (self-explanatory)

Second Card – The 11 parameters shown here specify: (1) cylindrical geometry; (2) 100 mesh intervals used in the previous XSDRNPM calculation; (3) the XSDRNPM calculation used an S_{12} quadrature; (4) the angular flux file written by XSDRNPM is found on logical unit number 16; (5) the cross-section library containing the appropriate multigroup flux-to-dose conversion factors is found on logical unit number 85; (6) that particular cross-section library is a "working" library; (7) calculate the local dose rate at four different points; (8) two dose factor IDs will be entered on the next data card; (9) use 200 increments in the numerical integration for the scalar flux; (10) radius of the cylinder is 99.005 cm; (11) the finite cylinder extends from z = 0.0 cm to z = 508 cm.

Third Card – Use the Straker-Morrison neutron flux-to-dose conversion factors (9028) for the neutrons, and the Straker-Morrison gamma-ray flux-to-dose conversion factors (9501) for the photons. Note: The ANSI Standard flux-to-dose conversion factors (9029 and 9504) would normally have been specified. Unfortunately, those flux-to-dose conversion factors were not available in this particular cross-section library at the time this sample problem was run.

Fourth Card – Given that the cylinder extends from z = 0 cm to z = 508 cm (see item 11 on the parameter card), the four detectors will be located at (r_1 = 99.005 cm, z_1 = 254 cm), (r_2 = 190.445 cm, z_2 = 254 cm), (r_3 = 304.8 cm, z_3 = 254 cm), and (r_4 = 304.8 cm, z_4 = 508 cm).

F4.5.4 XSDRNPM OUTPUT WITH EXPLANATORY COMMENTS

PB CASK CONTAINING 15 2-YEAR-OLD PWR FUEL ASSEMBLIES

GENERAL PROBLEM DESCRIPTION DATA BLOCK

GENERAL PROBLEM DATA

IGE	1/2/3 = PLANE/CYLINDER/SPHERE	2	ISN	QUADRATURE ORDER	12
IZM	NUMBER OF ZONES	6	ISCT	ORDER OF SCATTERING	3
IM	NUMBER OF SPACIAL INTERVALS	100	IEVT	0/1/2/3/4/5/6=Q/K/ALPHA/C/Z/R/H	0
IBL	0/1/2/3 = VACUUM/REFL/PER/WHITE	1	IIM	INNER ITERATION MAXIMUM	100
IBR	RIGHT BOUNDARY CONDITION	0	ICM	OUTER ITERATION MAXIMUM	20
MXX	NUMBER OF MIXTURES	4	ICLC	-1/0/N--FLAT RES/SN/OPT	0
MS	MIXING TABLE LENGTH	18	ITH	0/1 = FORWARD/ADJOINT	0
IGM	NUMBER OF ENERGY GROUPS	40	IFLU	NOT USED(ALWAYS WGTD)	3
NNG	NUMBER OF NEUTRON GROUPS	22	IPRT	-2/-1/0/N=MIXTURE XSEC PRINT	-1
NGG	NUMBER OF GAMMA GROUPS	18	ID1	0/1/2/3=NO/PRT ND/PCH N/BOTH	0
IFTG	NUMBER OF FIRST THERMAL GROUP	22	IPBT	-1/0/1=NONE/FINE/ALL BAL. PRT	0

SPECIAL OPTIONS

IFG	0/1 = NONE/WEIGHTING CALCULATION	0	IPN	0/1/2 DIFF. COEF. PARAM	0
ICM	VOLUMETRIC SOURCES (0/N=NO/YES)	1	IDFM	0/1 = NONE/DENSITY FACTORS 38*	0
IPM	BOUNDARY SOURCES (0/N=NO/YES)	0	IAZ	0/N = NONE/N ACTIVITIES BY ZONE	0
IFN	0/1/2 = INPUT 33*/34*/USE LAST	0	IAI	0/1=NONE/ACTIVITIES BY INTERVAL	0
ITMX	MAXIMUM TIME (MINUTES)	0	IFCT	0/1=NO/YES UPSCATTER SCALING	0
IDT1	0/1/2/3=NO/XSECT/SRCE/FLUX--OUT	0	IPVT	0/1/2=NO/K/ALPHA PARAMETRIC SRCH	0
ISX	BROAD GROUP FLUXES	0	ISEN	OUTER ITERATION ACCELERATION	0
IELN	ACTIVITY DATA UNIT	0	NBND	BAND REBALN PARAMETER	0

FLOATING POINT PARAMETERS

EPS	OVERALL CONVERGENCE	1.00000E-04	DY	CYL/PLA HT FOR BUCKLING	0.0
PTC	POINT CONVERGENCE	1.00000E-04	DZ	PLANE DEPTH FOR BUCKLING	0.0
XNF	NORMALIZATION FACTOR	8.80500E+14	VSC	VOID STREAMING CORRECTION	0.0
EV	EIGENVALUE GUESS	0.0	PV	IPVT=1/2--K/ALPHA	0.0
EVM	EIGENVALUE MODIFIER	0.0	EQL	EV CHANGE EPS FOR SEARCH	1.00000E-03
BF	BUCKLING FACTOR=1.420892	1.42089E+00	XNPM	NEW PARAM MOD FOR SEARCH	7.50000E-01

THIS CASE WILL REQUIRE 2281 LOCATIONS FOR MIXING
THIS CASE HAS BEEN ALLOCATED 139776 LOCATIONS

PB CASK CONTAINING 15 2-YEAR-OLD PWR FUEL ASSEMBLIES

13$ ARRAY 18 ENTRIES READ

14$ ARRAY 18 ENTRIES READ

15* ARRAY 18 ENTRIES READ

OT

DATA BLOCK 2 (MIXING TABLE, ETC.)

NUCLIDES ON TAPE	CCCC IDENTIFICATION
1 500000	
2 1001	
3 2004	
4 3006	
5 3007	
6 4009	
7 5010	
8 5011	
9 6012	
10 7014	
11 8016	
12 9019	
13 11023	
14 12000	
15 13027	
16 14028	
17 17000	
18 19039	
19 20040	
20 22000	
21 24000	
22 25055	
23 26000	
24 28000	
25 29000	
26 40000	
27 42000	
28 50000	
29 73181	
30 74000	
31 82000	
32 92235	
33 92238	
34 94239	
35 94240	

MIXING TABLE MIXTURE	COMPONENT	ATOM DENSITY	EXTRA XSECT ID'S
1	92235	3.11000E-05	
1	92238	3.65000E-03	
1	94239	1.94000E-05	
1	94240	8.84000E-06	
1	8016	7.41000E-03	
1	40000	2.12000E-03	
1	13027	2.46000E-02	
2	26000	5.94000E-02	
2	24000	1.74000E-02	
2	28000	7.72000E-03	
2	25055	1.74000E-03	
3	82000	3.30000E-02	
4	1001	6.41000E-02	
4	6012	1.42000E-02	
4	8016	2.60000E-02	
4	5010	1.15000E-04	
4	5011	4.96000E-04	
4	19039	3.05000E-04	

Mixing Table printed here is the same as that shown in Table F4.5.1 and entered using the 13$, 14$ and 15* Arrays.

MACROSCOPIC 1-D CROSS SECTIONS FOR MIXTURE 1

	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
Diff Coef → 1	5.91680E+00	5.69616E+00	5.90549E+00	6.06364E+00	5.83360E+00	5.26745E+00	4.61391E+00	4.52366E+00
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	4.93526E-04	1.94776E-03	5.82330E-03	1.91958E-02	3.97554E-02	5.13279E-02	1.08347E-01	8.72999E-02
Σ_F → 5	6.72602E-03	5.67098E-03	5.41677E-03	4.47737E-03	2.70730E-03	2.38083E-03	2.24140E-03	2.18069E-03
6	1.07257E-02	1.01454E-02	8.36802E-03	5.95761E-03	3.37142E-03	2.86048E-03	2.21493E-03	2.12304E-03
7	1.68150E-02	1.41775E-02	1.35420E-02	1.11935E-02	6.76824E-03	5.95208E-03	5.60348E-03	5.45173E-03
8	8.41429E-02	8.63295E-02	8.39972E-02	8.56525E-02	9.37610E-02	1.00859E-01	1.14676E-01	1.14549E-01

	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
1	4.84147E+00	4.17533E+00	3.55841E+00	2.75522E+00	1.91380E+00	1.81049E+00	2.35030E+00	1.67436E+00
Σ_{UPSCAT} → 2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	2.11063E-02	1.15414E-01	2.08856E-01	1.92547E-01	1.33604E-01	1.42610E-02	2.10620E-05	1.52617E-06
5	2.23599E-03	2.16522E-03	9.31647E-04	1.07547E-04	7.68849E-05	1.24889E-04	3.51431E-04	9.07329E-04
Σ_A → 6	2.22213E-03	2.22923E-03	1.26225E-03	6.64673E-04	6.95496E-04	2.43019E-03	8.30754E-03	3.55617E-02
7	5.58996E-03	5.41304E-03	2.32912E-03	2.68867E-04	1.92212E-04	3.12223E-04	8.78577E-04	2.26832E-03
8	1.02478E-01	1.22256E-01	1.34308E-01	1.62418E-01	1.98149E-01	1.89223E-01	1.45163E-01	2.04144E-01

	GRP. 17	GRP. 18	GRP. 19	GRP. 20	GRP. 21	GRP. 22	GRP. 23	GRP. 24
1	1.13725E+00	1.41839E+00	1.47057E+00	2.96503E+00	1.75515E+00	1.91558E+00	3.00747E+00	3.08924E+00
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\Sigma_{n,2n}$ → 3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	1.00621E-07	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	2.00336E-03	3.50431E-03	1.72585E-03	1.08756E-03	4.91037E-03	3.09762E-02	0.0	0.0
6	1.03784E-01	1.11915E-01	1.22313E-01	7.93492E-03	7.97676E-02	5.36536E-02	7.41877E-01	5.57452E-01
$\nu\Sigma_F$ → 7	5.00839E-03	8.76077E-03	4.31462E-03	2.71891E-03	1.22759E-02	7.74406E-02	0.0	0.0
8	2.96999E-01	2.40683E-01	2.30550E-01	1.16656E-01	1.94142E-01	1.74109E-01	1.13200E-01	1.10640E-01

	GRP. 25	GRP. 26	GRP. 27	GRP. 28	GRP. 29	GRP. 30	GRP. 31	GRP. 32
1	3.12295E+00	3.06997E+00	3.03525E+00	2.83812E+00	2.71223E+00	2.47750E+00	2.27846E+00	1.99633E+00
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
X(SPEC) → 4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	4.19888E-01	3.14858E-01	2.37449E-01	1.85544E-01	1.55670E-01	1.34383E-01	1.20633E-01	1.10611E-01
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Σ_T → 8	1.11018E-01	1.13269E-01	1.17396E-01	1.23751E-01	1.32129E-01	1.44100E-01	1.59878E-01	1.88381E-01

	GRP. 33	GRP. 34	GRP. 35	GRP. 36	GRP. 37	GRP. 38	GRP. 39	GRP. 40
1	1.61162E+00	1.32326E+00	9.26911E-01	5.29203E-01	2.71910E-01	9.21954E-02	4.53908E-02	4.10359E-03
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	1.05637E-01	1.07633E-01	1.25959E-01	1.73594E-01	2.74504E-01	5.67984E-01	1.14062E+00	1.04716E+01
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	2.28806E-01	2.85948E-01	4.17492E-01	6.89657E-01	1.31656E+00	3.70353E+00	7.40089E+00	8.12497E+01

*See note on following page regarding $\Sigma_{n,2n}$, Σ_A, and the P_3 representation of the scattering cross section.

For brevity, the next 5-6 pages of output have not been included here.

*The SCALE 22n-18Y working library was used for this shielding calculation. It is an older cross section library, corresponding to the popular DLC-23/CASK library distributed by the Radiation Shielding and Information Center at Oak Ridge.

*The (n,2n) data is generally found two different places in an AMPX working library: in the (2-D) group-to-group transfer arrays, and in the (1-D) cross section array that summarizes that data. The (1-D) summary array is only used to generate and print balance tables. In this particular library, the (1-D) summary array for the (n,2n) data was simply set to zero. The (2-D) transfer arrays used in the transport calculation are OK however.

*While Σ_A is used to generate and print balance tables for each zone, it is not used in the actual transport calculation for the flux. In this particular library, the absorption cross section in groups 23-40 was really replaced by the kerma factor for the associated gamma group so that $\phi\Sigma_A$ would yield the corresponding energy deposition rate. While this will mess-up the balance tables printed below, it will not affect the actual flux solution.

*With each group-to-group transfer there is an associated angular distribution, $\sigma_s^{g' \to g}(\mu)$. In this particular library, each group-to-group transfer is represented by a P_3 Legendre expansion in μ:

$$\sigma_s^{g' \to g}(\mu) = \sum_{n=0}^{3} \sigma_n^{g' \to g} P_n(\mu)$$

While the actual scattering distributions are obviously greater than (or equal to) zero for all μ ($-1 \leq \mu \leq +1$), the P_3 Legendre approximation may be negative for some values of μ. As a result, the XSDRNPM discrete ordinates calculation may generate negative fluxes for a few angular directions (μ_m) in some energy groups. (Indeed, as shown in the XSDOSE output below, XSDRNPM did generate a few negative angular fluxes on the surface of this particular cask). Generally these are quite small and/or in directions that are relatively unimportant in the shielding calculation. Using a P_1 approximation often eliminates this problem but, because it cannot adequately model the forward-directed scattering in many of the higher energy groups, such a low-order approximation could cause the user to underestimate the dose at the surface of the cask by a factor of two. Using a P_5 or P_7 approximation for the scattering kernel (if that data were available) would certainly tend to eliminate the occurance of negative angular fluxes but may do very little to improve the calculated dose at the surface.

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	MIXTURE BY ZONE	ORDER P(L) BY ZONE	ACTIVITY TABLE MATL NO.	ACTIVITY TABLE REACTION	QUADRATURE CONSTANTS WEIGHTS	DIRECTIONS	REFL DIREC	WT X COS
1	1	3			0	-1.91151E-01	3	0
2	2	3			2.35877E-02	-1.35164E-01	3	-3.18821E-03
3	3	3			2.35877E-02	1.35164E-01	2	3.18821E-03
4	2	3			0	-4.27285E-01	8	0
5	4	3			2.67348E-02	-3.94759E-01	8	-1.05538E-02
6	2	3			2.67348E-02	-1.63514E-01	7	-4.37152E-03
7					2.67348E-02	1.63515E-01	6	4.37154E-03
8					2.67348E-02	3.94759E-01	5	1.05538E-02
9					0	-6.38161E-01	15	0
10					2.66797E-02	-6.16416E-01	15	-1.64458E-02
11					2.66797E-02	-4.51248E-01	14	-1.20392E-02
12					2.66797E-02	-1.65167E-01	13	-4.40661E-03
13					2.66797E-02	1.65169E-01	12	4.40665E-03
14					2.66797E-02	4.51248E-01	11	1.20392E-02
15					2.66797E-02	6.16417E-01	10	1.64458E-02
16					0	-8.09356E-01	24	0
17	All these belong to "eta level number 4"				2.53959E-02	-7.93805E-01	24	-2.01594E-02
18	μ_m are listed in column labeled DIRECTIONS				2.53959E-02	-6.72954E-01	23	-1.70903E-02
19					2.53959E-02	-4.49654E-01	22	-1.14194E-02
20					2.53959E-02	-1.57897E-01	21	-4.00994E-03
21					2.53959E-02	1.57898E-01	20	4.00997E-03
22	$\eta_m = \sqrt{1.0 - \mu_{16}^2} = 0.344943$ m=16,...,24				2.53959E-02	4.49654E-01	19	1.14194E-02
23					2.53959E-02	6.72955E-01	18	1.70903E-02
24					2.53959E-02	7.93805E-01	17	2.01594E-02
25					0	-9.29892E-01	35	0
26					2.33492E-02	-9.18444E-01	35	-2.14450E-02
27					2.33492E-02	-8.28540E-01	34	-1.93458E-02
28					2.33492E-02	-6.57533E-01	33	-1.53529E-02
29					2.33492E-02	-4.22161E-01	32	-9.85715E-03
30					2.33492E-02	-1.45466E-01	31	-3.39652E-03
31					2.33492E-02	1.45468E-01	30	3.39658E-03
32					2.33492E-02	4.22163E-01	29	9.85720E-03
33					2.33492E-02	6.57533E-01	28	1.53529E-02
34					2.33492E-02	8.28540E-01	27	1.93458E-02
35					2.33492E-02	9.18444E-01	26	2.14450E-02
36					0	-9.92127E-01	48	0
37					2.07622E-02	-9.83639E-01	48	-2.04226E-02
38					2.07622E-02	-9.16605E-01	47	-1.90308E-02
39					2.07622E-02	-7.87107E-01	46	-1.63421E-02
40					2.07622E-02	-6.03968E-01	45	-1.25397E-02
41					2.07622E-02	-3.79670E-01	44	-7.88279E-03
42					2.07622E-02	-1.29497E-01	43	-2.68865E-03
43					2.07622E-02	1.29499E-01	42	2.68870E-03
44					2.07622E-02	3.79671E-01	41	7.88282E-03
45					2.07622E-02	6.03969E-01	40	1.25398E-02
46					2.07622E-02	7.87108E-01	39	1.63421E-02
47					2.07622E-02	9.16606E-01	38	1.90308E-02
48					2.07622E-02	9.83640E-01	37	2.04226E-02

Note that an S_{12} quadrature in cylindrical geometry has 48 discrete directions and that this same quadrature set will later be used by XSDOSE.

For brevity, the next 1-2 pages of output have not been included here.

VOLUMETRIC SOURCE SPECTRA

GRP.	SPEC 1
1	4.30849E-02
2	3.66321E-01
3	1.00730E+00
4	5.02988E+00
5	1.27071E+01
6	1.79289E+01
7	5.04311E+01
8	4.02721E+01
9	9.38138E+00
10	4.64933E+01
11	7.88896E+01
12	6.89953E+01
13	3.17941E+01
14	1.56423E-03
15	0.0
	GRP. 16 THRU GRP. 22 SAME AS ABOVE
23	1.87793E-01
24	1.2257CE+00
25	7.49518E+00
26	7.08815E+00
27	2.33525E+05
28	1.86867E+06
29	1.03443E+08
30	4.38129E+07
31	5.47330E+08
32	1.02252E+09
33	3.14036E+09
34	7.58783E+09
35	9.56338E+09
36	1.05925E+09
37	1.91334E+09
38	4.55336E+09
39	7.09146E+09
40	3.44149E+10

For brevity, the next 1-2 pages of output have not been included below.

The volumetric source spectra edited here is the actual source used by the code; that is:

$X_i \equiv$ volumetric source for group i in the fixed source calculation (particles/sec)/cm^3

$$X_i = \frac{S^i}{V} = \left(\frac{N_A}{L_F A}\right) X_i = \left(\frac{XNF}{S_A^n + S_A^\gamma}\right)\left(\frac{X_i}{A}\right) = \left[\frac{XNF}{\sum_{j=1}^{22} X_j + \sum_{j=23}^{40} X_j}\right]\left(\frac{X_i}{A}\right)$$

where N_A is the number of assemblies

L_F is the active length of the fuel

A is the area of the source region (πR_F^2)

S_A^n is the total neutron source per assembly

S_A^γ is the total gamma source per assembly

and X_i is the spectra as calculated for (and entered in) the 31* Array.

In general, XSDRNPM will calculate these values (X_i) as

$$X_i = \left(\frac{XNF}{A}\right)\left[\frac{X_i}{\sum_{j=1}^{40} X_j}\right]$$

where $A = \pi \sum_k (r_{k+1}^2 - r_k^2)$

and k is summed over all mesh intervals containing "volumetric source spectra number 1" (see the input for the 30$ Array).

In this particular case, $A=\pi(62.81cm)^2$

and $\sum_{j=1}^{40} X_j = S_A^n + S_A^\gamma = 2.147 \times 10^{16}$, such that

$$X_i = \left[\frac{8.805(+14)}{1.239(+4)}\right]\left[\frac{X_i}{2.147(+16)}\right] = \left(3.310 \times 10^{-6}\right) X_i$$

OUTER ITER	INNER ITERS	1 - BALANCE	EIGENVALUE	1 - SOURCE RATIO	1 - SCATTER RATIO	1 - UPSCAT RATIO	SEARCH PARAMETER	TIME (MIN)
1	356	4.94282E-07	1.97249D-01	-1.00878E-09	1.00000E+00	0.0	0.0	1.3660
2	572	4.94281E-07	1.96502D-01	-1.94403E-10	-1.96045E-08	0.0	0.0	2.1888

These numbers should all become small as the problem converges.

GRP TO GRP	INNER ITERS	MFD INT.	MAX. FLUX DIFFERENCE	MSF INT.	MAX. SCALE FACTOR	COARSE MESH
1	7	93	6.00734D-05	100	9.99981D-01	11
2	5	95	9.17920D-05	74	1.00003D+00	11
3	6	88	7.83180D-05	100	9.99962D-01	12
4	5	95	8.94542D-05	100	9.99963D-01	12
5	5	31	8.86668D-05	45	1.00005D+00	13
6	5	30	7.01784D-05	81	9.99946D-01	15
7	5	31	7.38018D-05	100	9.99947D-01	15
8	5	31	6.73238D-05	45	1.00004D+00	15
9	5	82	5.18475D-05	74	9.99989D-01	14
10	5	31	3.25490D-05	48	1.00002D+00	14
11	4	32	9.59262D-05	68	1.00008D+00	17
12	4	32	5.03585D-05	100	1.00004D+00	18
13	4	99	5.74547D-05	100	1.00006D+00	27
14	5	85	4.75584D-05	3	1.00006D+00	36
15	5	99	8.43974D-05	100	1.00004D+00	37
16	7	81	5.73535D-05	80	1.00008D+00	41
17	5	99	8.24348D-05	54	1.00004D+00	40
18	5	99	9.53210D-05	54	1.00005D+00	40
19	5	99	9.09662D-05	63	1.00005D+00	40
20	5	99	9.72386D-05	77	1.00005D+00	35
21	6	99	3.81672D-05	77	1.00002D+00	41
22	7	97	4.49287D-05	62	1.00001D+00	37
23	3	51	4.86625D-06	56	1.00000D+00	16
24	3	82	4.79955D-06	100	1.00000D+00	15
25	3	100	8.07582D-06	53	1.00000D+00	15
26	3	39	1.17321D-05	53	1.00000D+00	15
27	3	88	1.91666D-05	100	9.99999D-01	16
28	2	80	6.39906D-05	100	9.99998D-01	16
29	2	91	1.41339D-05	100	1.00000D+00	18
30	2	85	5.91904D-06	99	1.00000D+00	19
31	2	36	2.86227D-05	98	1.00000D+00	20
32	1	99	8.93634D-05	100	1.00002D+00	22
33	1	99	9.39293D-05	100	1.00002D+00	28
34	1	98	9.19871D-05	100	1.00003D+00	33
35	3	95	3.67605D-05	100	9.99991D-01	53
36	2	83	7.50997D-05	93	9.99993D-01	74
37	2	82	7.09615D-05	100	1.00002D+00	76
38	3	81	1.92519D-05	97	1.00001D+00	77
39	3	98	2.11942D-05	95	1.00001D+00	87
40	3	97	4.96218D-06	97	1.00000D+00	92

Generation-to-generation neutron multiplication factor (k) for this particular fixed-source problem. Because the dry, homogenized fuel in Zone 1 was depleted, this value is quite small and only 3 outer (spectral) iterations were required. In problems where this is close to 1.0, many outer iterations may be required.

3	729	4.94281E-07	1.96438D-01	-3.77909E-11	-2.06262E-09	0.0	0.0	2.7988

FINAL MONITOR LAMBDA 1.00000E+00

ANGULAR FLUX ON 16

Later, XSDOSE will read these angular fluxes on logical unit 16.

ELAPSED TIME 2.80 MIN.

For brevity, the next 1-2 pages of output have not been included below.

PB CASK CONTAINING 15 2-YEAR-OLD PWR FUEL ASSEMBLIES

TOTAL FLUX

INT.	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
1	1.82527E+00	1.12988E+01	3.52134E+01	1.65269E+02	4.27082E+02	5.92855E+02	1.68047E+03	1.78854E+03
2	1.82371E+00	1.12912E+01	3.51880E+01	1.65157E+02	4.26797E+02	5.92487E+02	1.67953E+03	1.78742E+03
3	1.82051E+00	1.12756E+01	3.51353E+01	1.64925E+02	4.26214E+02	5.91737E+02	1.67764E+03	1.78517E+03
4	1.81575E+00	1.12525E+01	3.50572E+01	1.64580E+02	4.25350E+02	5.90621E+02	1.67481E+03	1.78180E+03
5	1.80939E+00	1.12214E+01	3.49524E+01	1.64118E+02	4.24188E+02	5.89117E+02	1.67097E+03	1.77723E+03
6	1.80135E+00	1.11820E+01	3.48196E+01	1.63532E+02	4.22713E+02	5.87197E+02	1.66605E+03	1.77138E+03
7	1.79151E+00	1.11335E+01	3.46565E+01	1.62811E+02	4.20895E+02	5.84827E+02	1.65994E+03	1.76411E+03
8	1.77977E+00	1.10753E+01	3.44609E+01	1.61945E+02	4.18705E+02	5.81963E+02	1.65251E+03	1.75528E+03
9	1.76596E+00	1.10064E+01	3.42295E+01	1.60918E+02	4.16104E+02	5.78552E+02	1.64361E+03	1.74472E+03
10	1.74989E+00	1.09255E+01	3.39587E+01	1.59712E+02	4.13046E+02	5.74523E+02	1.63303E+03	1.73217E+03
11	1.73135E+00	1.08313E+01	3.36438E+01	1.58307E+02	4.09475E+02	5.69796E+02	1.62052E+03	1.71738E+03
12	1.71004E+00	1.07219E+01	3.32791E+01	1.56674E+02	4.05315E+02	5.64271E+02	1.60579E+03	1.70000E+03
13	1.68564E+00	1.05951E+01	3.28577E+01	1.54781E+02	4.00482E+02	5.57827E+02	1.58848E+03	1.67964E+03
14	1.65773E+00	1.04482E+01	3.23709E+01	1.52587E+02	3.94870E+02	5.50304E+02	1.56810E+03	1.65578E+03
15	1.62578E+00	1.02776E+01	3.18081E+01	1.50041E+02	3.88347E+02	5.41516E+02	1.54410E+03	1.62781E+03
16	1.58915E+00	1.00790E+01	3.11558E+01	1.47081E+02	3.80748E+02	5.31221E+02	1.51575E+03	1.59497E+03
17	1.54700E+00	9.84663E+00	3.03965E+01	1.43622E+02	3.71854E+02	5.19118E+02	1.48216E+03	1.55635E+03
18	1.49824E+00	9.57276E+00	2.95072E+01	1.39557E+02	3.61385E+02	5.04792E+02	1.44209E+03	1.51070E+03
19	1.44143E+00	9.24742E+00	2.84584E+01	1.34746E+02	3.48980E+02	4.87723E+02	1.39401E+03	1.45651E+03
20	1.37444E+00	8.85548E+00	2.72057E+01	1.28982E+02	3.34101E+02	4.67130E+02	1.33560E+03	1.39161E+03
21	1.29456E+00	8.37774E+00	2.56929E+01	1.22000E+02	3.16077E+02	4.42048E+02	1.26410E+03	1.31336E+03
22	1.19595E+00	7.77325E+00	2.38033E+01	1.13256E+02	2.93514E+02	4.10441E+02	1.17348E+03	1.21654E+03
23	1.07186E+00	6.99512E+00	2.13964E+01	1.02101E+02	2.64884E+02	3.70308E+02	1.05897E+03	1.09659E+03
24	8.69360E-01	5.68552E+00	1.74796E+01	8.39343E+01	2.18511E+02	3.04578E+02	8.71484E+02	9.13984E+02
25	6.64801E-01	4.33228E+00	1.33827E+01	6.42712E+01	1.68381E+02	2.33720E+02	6.75152E+02	7.31476E+02
26	5.46294E-01	3.53852E+00	1.08747E+01	5.16597E+01	1.36193E+02	1.88931E+02	5.55771E+02	6.19763E+02
27	4.63400E-01	2.99183E+00	9.16562E+00	4.31967E+01	1.14447E+02	1.58707E+02	4.72665E+02	5.37771E+02
28	3.99760E-01	2.57350E+00	7.86028E+00	3.67663E+01	9.78154E+01	1.35626E+02	4.08050E+02	4.71851E+02
29	3.48218E-01	2.23454E+00	6.80487E+00	3.15938E+01	8.44021E+01	1.17089E+02	3.55443E+02	4.16810E+02
30	3.05126E-01	1.95044E+00	5.92438E+00	2.73102E+01	7.33250E+01	1.01923E+02	3.11881E+02	3.70218E+02
31	2.68315E-01	1.70579E+00	5.17178E+00	2.36890E+01	6.41082E+01	8.96150E+01	2.76089E+02	3.31050E+02
32	2.44864E-01	1.54875E+00	4.69081E+00	2.14328E+01	5.84212E+01	8.23011E+01	2.55230E+02	3.08589E+02
33	2.32465E-01	1.46625E+00	4.43805E+00	2.03003E+01	5.54885E+01	7.86324E+01	2.45508E+02	2.99148E+02
34	2.20834E-01	1.39001E+00	4.20463E+00	1.92464E+01	5.27012E+01	7.50298E+01	2.35804E+02	2.89662E+02
35	2.09903E-01	1.31912E+00	3.98773E+00	1.82614E+01	5.00588E+01	7.15417E+01	2.26291E+02	2.80279E+02
36	1.99614E-01	1.25293E+00	3.78525E+00	1.73378E+01	4.75569E+01	6.81904E+01	2.17055E+02	2.71082E+02
37	1.89919E-01	1.19092E+00	3.59562E+00	1.64699E+01	4.51894E+01	6.49850E+01	2.08139E+02	2.62114E+02
38	1.80773E-01	1.13268E+00	3.41755E+00	1.56528E+01	4.29497E+01	6.19270E+01	1.99561E+02	2.53401E+02
39	1.72138E-01	1.07788E+00	3.25004E+00	1.48827E+01	4.08307E+01	5.90142E+01	1.91325E+02	2.44952E+02
40	1.63979E-01	1.02624E+00	3.09221E+00	1.41560E+01	3.88256E+01	5.62417E+01	1.83427E+02	2.36770E+02
41	1.56264E-01	9.77509E-01	2.94329E+00	1.34696E+01	3.69275E+01	5.36039E+01	1.75857E+02	2.28853E+02
42	1.48964E-01	9.31477E-01	2.80263E+00	1.28207E+01	3.51302E+01	5.10947E+01	1.68606E+02	2.21196E+02
43	1.42051E-01	8.87950E-01	2.66966E+00	1.22069E+01	3.34277E+01	4.87075E+01	1.61661E+02	2.13793E+02
44	1.35503E-01	8.46761E-01	2.54384E+00	1.16259E+01	3.18143E+01	4.64369E+01	1.55009E+02	2.06636E+02
45	1.29295E-01	8.07756E-01	2.42472E+00	1.10756E+01	3.02849E+01	4.42766E+01	1.48636E+02	1.99718E+02
46	1.23408E-01	7.70794E-01	2.31186E+00	1.05541E+01	2.88343E+01	4.22208E+01	1.42534E+02	1.93026E+02
47	1.17822E-01	7.35746E-01	2.20487E+00	1.00597E+01	2.74583E+01	4.02640E+01	1.36688E+02	1.86561E+02
48	1.12519E-01	7.02495E-01	2.10338E+00	9.59070E+00	2.61524E+01	3.84010E+01	1.31087E+02	1.80312E+02
49	1.07482E-01	6.70932E-01	2.00707E+00	9.14561E+00	2.49126E+01	3.66270E+01	1.25719E+02	1.74269E+02
50	1.02696E-01	6.40957E-01	1.91563E+00	8.72302E+00	2.37351E+01	3.49373E+01	1.20574E+02	1.68425E+02
51	9.81463E-02	6.12477E-01	1.82877E+00	8.32167E+00	2.26164E+01	3.33274E+01	1.15642E+02	1.62773E+02
52	9.38201E-02	5.85408E-01	1.74623E+00	7.94035E+00	2.15532E+01	3.17933E+01	1.10913E+02	1.57307E+02
53	8.97046E-02	5.59668E-01	1.66777E+00	7.57790E+00	2.05426E+01	3.03310E+01	1.06378E+02	1.52018E+02
54	8.57881E-02	5.35183E-01	1.59315E+00	7.23328E+00	1.95815E+01	2.89369E+01	1.02028E+02	1.46901E+02
55	8.20597E-02	5.11883E-01	1.52217E+00	6.90548E+00	1.86673E+01	2.76073E+01	9.78537E+01	1.41948E+02

After obtaining a solution, the user should inspect these results to verify that there is no energy group in which the scalar flux changes by more than 50-60% as one goes from one mesh interval to the next. If that were the case, more mesh intervals may be warranted.

56	7.85091E-02	4.89704E-01	1.45462E+00	6.59358E+00	1.77973E+01	2.63382E+01	9.38479E+01	1.37154E+02
57	7.51268E-02	4.68586E-01	1.39031E+00	6.29673E+00	1.69693E+01	2.51280E+01	9.00028E+01	1.32512E+02
58	7.19040E-02	4.48474E-01	1.32907E+00	6.01412E+00	1.61810E+01	2.39730E+01	8.63084E+01	1.28017E+02
59	6.88323E-02	4.29314E-01	1.27075E+00	5.74498E+00	1.54302E+01	2.28703E+01	8.27628E+01	1.23663E+02
60	6.59041E-02	4.11055E-01	1.21517E+00	5.48859E+00	1.47146E+01	2.18173E+01	7.93566E+01	1.19440E+02
61	6.31118E-02	3.93653E-01	1.16220E+00	5.24429E+00	1.40331E+01	2.08112E+01	7.60833E+01	1.15352E+02
62	6.04485E-02	3.77063E-01	1.11171E+00	5.01143E+00	1.33834E+01	1.98497E+01	7.29364E+01	1.11387E+02
63	5.79078E-02	3.61245E-01	1.06356E+00	4.78943E+00	1.27639E+01	1.89303E+01	6.99098E+01	1.07542E+02
64	5.54837E-02	3.46162E-01	1.01764E+00	4.57774E+00	1.21730E+01	1.80509E+01	6.69977E+01	1.03811E+02
65	5.31704E-02	3.31778E-01	9.73832E-01	4.37582E+00	1.16091E+01	1.72092E+01	6.41941E+01	1.00188E+02
66	5.09628E-02	3.18061E-01	9.32033E-01	4.18319E+00	1.10707E+01	1.64030E+01	6.14930E+01	9.66680E+01
67	4.88560E-02	3.04981E-01	8.92145E-01	3.99932E+00	1.05566E+01	1.56303E+01	5.88884E+01	9.32441E+01
68	4.68455E-02	2.92511E-01	8.54075E-01	3.82394E+00	1.00651E+01	1.48886E+01	5.63738E+01	8.99097E+01
69	4.49272E-02	2.80628E-01	8.17736E-01	3.65657E+00	9.59514E+00	1.41752E+01	5.39419E+01	8.66562E+01
70	4.30979E-02	2.69311E-01	7.83053E-01	3.49689E+00	9.14522E+00	1.34882E+01	5.15841E+01	8.34734E+01
71	4.13547E-02	2.58547E-01	7.49955E-01	3.34463E+00	8.71399E+00	1.28240E+01	4.92882E+01	8.03471E+01
72	3.96956E-02	2.48325E-01	7.18380E-01	3.19957E+00	8.29989E+00	1.21779E+01	4.70414E+01	7.72570E+01
73	3.81199E-02	2.38644E-01	6.88277E-01	3.06165E+00	7.90116E+00	1.15436E+01	4.48196E+01	7.41722E+01
74	3.53592E-02	2.21890E-01	6.37437E-01	2.81952E+00	7.20735E+00	1.04081E+01	4.05348E+01	6.75162E+01
75	3.15691E-02	1.98713E-01	5.68075E-01	2.48507E+00	6.27845E+00	8.91760E+00	3.47607E+01	5.81994E+01
76	2.81660E-02	1.77522E-01	5.04940E-01	2.18370E+00	5.47195E+00	7.67908E+00	2.99543E+01	5.03825E+01
77	2.51221E-02	1.58404E-01	4.48232E-01	1.91629E+00	4.76847E+00	6.62226E+00	2.58396E+01	4.36277E+01
78	2.23997E-02	1.41225E-01	3.97501E-01	1.67991E+00	4.15290E+00	5.71177E+00	2.22743E+01	3.77104E+01
79	1.99602E-02	1.25795E-01	3.52140E-01	1.47084E+00	3.61202E+00	4.92158E+00	1.91566E+01	3.24636E+01
80	1.77650E-02	1.11910E-01	3.11484E-01	1.28508E+00	3.13273E+00	4.22833E+00	1.63897E+01	2.77125E+01
81	1.57707E-02	9.93479E-02	2.74736E-01	1.11699E+00	2.69471E+00	3.59949E+00	1.38278E+01	2.31345E+01
82	1.41167E-02	8.86998E-02	2.43563E-01	9.74154E-01	2.31357E+00	3.04971E+00	1.13783E+01	1.85997E+01
83	1.27977E-02	7.99320E-02	2.18129E-01	8.59867E-01	2.00881E+00	2.61003E+00	9.31069E+00	1.48446E+01
84	1.16287E-02	7.21967E-02	1.96027E-01	7.63324E-01	1.75929E+00	2.25628E+00	7.74665E+00	1.21544E+01
85	1.05831E-02	6.53158E-02	1.76558E-01	6.79888E-01	1.54787E+00	1.96014E+00	6.49000E+00	1.00557E+01
86	9.64291E-03	5.91641E-02	1.59277E-01	6.06932E-01	1.36580E+00	1.70816E+00	5.46055E+00	8.36889E+00
87	8.79472E-03	5.36462E-02	1.43864E-01	5.42705E-01	1.20768E+00	1.49195E+00	4.60937E+00	6.99421E+00
88	8.02777E-03	4.86853E-02	1.30075E-01	4.85920E-01	1.06962E+00	1.30550E+00	3.90156E+00	5.86495E+00
89	7.33321E-03	4.42177E-02	1.17708E-01	4.35568E-01	9.48662E-01	1.14416E+00	3.31051E+00	4.93225E+00
90	6.70347E-03	4.01892E-02	1.06603E-01	3.90821E-01	8.42407E-01	1.00416E+00	2.81537E+00	4.15880E+00
91	6.13204E-03	3.65528E-02	9.66132E-02	3.50990E-01	7.48890E-01	8.82424E-01	2.39952E+00	3.51546E+00
92	5.61325E-03	3.32675E-02	8.76179E-02	3.15488E-01	6.66467E-01	7.76405E-01	2.04961E+00	2.97933E+00
93	5.14217E-03	3.02970E-02	7.95093E-02	2.83810E-01	5.93774E-01	6.83992E-01	1.75495E+00	2.53237E+00
94	4.71453E-03	2.76099E-02	7.21921E-02	2.55543E-01	5.29699E-01	6.03487E-01	1.50713E+00	2.16088E+00
95	4.32682E-03	2.51754E-02	6.55769E-02	2.30321E-01	4.73423E-01	5.33701E-01	1.30037E+00	1.85652E+00
96	3.97613E-03	2.29640E-02	5.95746E-02	2.07855E-01	4.24664E-01	4.74496E-01	1.13531E+00	1.62409E+00
97	3.66595E-03	2.10588E-02	5.44812E-02	1.89388E-01	3.86471E-01	4.28483E-01	1.02000E+00	1.47917E+00
98	3.38644E-03	1.94133E-02	5.01248E-02	1.73714E-01	3.54323E-01	3.89254E-01	9.27757E-01	1.36650E+00
99	3.12233E-03	1.78697E-02	4.59654E-02	1.58290E-01	3.21144E-01	3.48656E-01	8.28441E-01	1.22909E+00
100	2.87169E-03	1.64054E-02	4.19415E-02	1.42963E-01	2.86752E-01	3.06081E-01	7.20786E-01	1.06978E+00

For brevity, the next 18 pages of output have not been included below.

FINE GROUP SUMMARY FOR ZONE 6 BY GROUP INCLUDING SUM FOR ALL GROUPS IN LINE 41

GRP.	FIX SOURCE	FISS SOURCE	IN SCATTER	SLF SCATTER	OUT SCATTER	ABSORPTION	LEAKAGE	BALANCE
1	0.0	0.0	0.0	4.09041E-01	4.67096E-01	7.17244E-02	-4.53267E-01	0.0
2	0.0	0.0	3.31563E-02	2.88186E+00	2.31331E+00	3.51927E-01	-2.61575E+00	8.02422E-01
3	0.0	0.0	2.26957E-01	8.60724E+00	6.48599E+00	6.57289E-01	-6.91550E+00	9.98176E-01
4	0.0	0.0	7.81322E-01	3.34231E+01	2.43031E+01	1.58213E+00	-2.51028E+01	9.99236E-01
5	0.0	0.0	3.33572E+00	7.41167E+01	4.87792E+01	2.16243E+00	-4.76066E+01	1.00010E+00
6	0.0	0.0	8.86163E+00	7.89873E+01	5.69651E+01	1.64942E+00	-4.97571E+01	1.00024E+00
7	0.0	0.0	2.11408E+01	1.91266E+02	1.17565E+02	2.19163E+00	-9.86228E+01	1.00017E+00
8	0.0	0.0	3.74988E+01	2.90528E+02	1.57099E+02	1.95809E+00	-1.21563E+02	1.00006E+00
9	0.0	0.0	4.11756E+01	6.43235E+01	7.69603E+01	3.70113E-01	-3.61526E+01	9.99974E-01
10	0.0	0.0	1.05334E+02	5.10614E+02	2.28730E+02	1.50217E+00	-1.24888E+02	9.99950E-01
11	0.0	0.0	2.71026E+02	1.32647E+03	3.62140E+02	2.47308E+00	-9.35806E+01	9.99988E-01
12	0.0	0.0	3.49738E+02	2.61760E+03	2.32163E+02	4.73478E+00	1.12743E+02	1.00014E+00
13	0.0	0.0	4.24938E+02	6.42867E+03	1.13461E+02	1.01934E+01	3.01050E+02	1.00028E+00
14	0.0	0.0	1.62149E+02	2.05630E+04	2.14660E+02	4.62933E+01	-9.92827E+01	1.00148E+00
15	0.0	0.0	2.15702E+02	1.13939E+04	2.05150E+02	1.35221E+02	-1.24766E+02	1.00022E+00
16	0.0	0.0	2.05295E+02	1.65090E+04	2.40825E+02	1.44455E+02	-1.79476E+02	9.98763E-01
17	0.0	0.0	2.40832E+02	9.93265E+03	2.55798E+02	6.71066E+01	-8.22263E+01	1.00032E+00
18	0.0	0.0	2.55799E+02	7.30080E+03	2.77587E+02	8.62552E+01	-1.07827E+02	9.99577E-01
19	0.0	0.0	2.77588E+02	9.26932E+03	2.81012E+02	1.90734E+02	-1.94127E+02	9.99945E-01
20	0.0	0.0	2.81012E+02	7.39129E+03	2.72181E+02	2.65772E+02	-2.56879E+02	9.99889E-01
21	0.0	0.0	2.72181E+02	6.78848E+03	2.49584E+02	4.01349E+02	-3.78853E+02	1.00019E+00
22	0.0	0.0	2.49584E+02	9.78804E+03	0.0	2.48353E+03	-2.23414E+03	1.00039E+00
23	0.0	0.0	7.44277E+02	1.03800E+02	5.34868E+03	2.58591E+04	-2.85041E+03	5.11502E-02
24	0.0	0.0	1.95203E+03	3.03573E+02	1.26381E+04	4.98847E+04	-7.07659E+03	6.80172E-02
25	0.0	0.0	1.60695E+03	2.61013E+02	6.61187E+03	2.11187E+04	-3.41382E+03	1.23976E-01
26	0.0	0.0	1.32141E+03	1.65692E+02	3.74095E+03	9.42585E+03	-1.72480E+03	2.07063E-01
27	0.0	0.0	1.83996E+03	5.86254E+02	7.95431E+03	1.59931E+04	-5.07494E+03	1.77668E-01
28	0.0	0.0	1.65915E+03	1.31827E+03	2.25312E+04	3.47918E+04	-1.90986E+04	8.31999E-02
29	0.0	0.0	4.54283E+03	5.98780E+04	7.11308E+05	9.05903E+05	-6.74405E+05	9.59063E-03
30	0.0	0.0	9.02919E+04	5.48032E+04	6.74017E+05	6.79597E+05	-5.70622E+05	2.06787E-01
31	0.0	0.0	1.99162E+05	1.53782E+05	1.39426E+06	1.14032E+06	-1.19131E+06	2.58244E-01
32	0.0	0.0	5.24777E+05	3.20531E+05	1.95001E+06	1.22659E+06	-1.43508E+06	4.63114E-01
33	0.0	0.0	7.35756E+05	2.43754E+05	1.66309E+06	7.39569E+05	-9.39842E+05	6.69303E-01
34	0.0	0.0	1.24186E+06	4.83817E+05	2.19124E+06	7.47751E+05	-9.78988E+05	7.75710E-01
35	0.0	0.0	2.42746E+06	1.34746E+06	3.41054E+06	8.62790E+05	-1.09667E+06	8.66312E-01
36	0.0	0.0	2.66973E+06	9.61375E+05	2.81496E+06	4.53191E+05	-3.47636E+05	9.55140E-01
37	0.0	0.0	4.93209E+06	2.48254E+06	3.88346E+06	5.86762E+05	2.25738E+05	1.02452E+00
38	0.0	0.0	5.92377E+06	7.08503E+06	2.29515E+06	9.82567E+05	-1.82950E+06	1.60710E+00
39	0.0	0.0	2.29527E+06	9.32258E+05	1.16277E+05	2.91752E+05	-2.07235E+06	7.27561E+00
40	0.0	0.0	1.16298E+05	1.15093E+03	0.0	2.62322E+03	-3.77131E+04	2.86419E+00
41	0.0	0.0	2.11735E+07	1.42397E+07	2.11665E+07	8.78033E+06	-1.09915E+07	1.05527E+00

GRP.	RT BDY FLUX	RT LEAKAGE	LFT BDY FLUX	LFT LEAKAGE	N2N RATE	FISS RATE	FLUX*D8**2	TOTAL FLUX
1	2.74955E-03	1.41636E+00	3.80981E-03	1.86962E+00	0.0	0.0	0.0	3.82604E+00
2	1.56908E-02	7.99717E+00	2.19104E-02	1.06129E+01	0.0	0.0	0.0	2.19205E+01
3	3.99559E-02	2.00513E+01	5.67168E-02	2.69668E+01	0.0	0.0	0.0	5.64553E+01
4	1.35279E-01	6.67465E+01	1.97286E-01	9.18493E+01	0.0	0.0	0.0	1.94818E+02
5	2.69098E-01	1.28307E+02	4.02185E-01	1.75913E+02	0.0	0.0	0.0	3.95481E+02
6	2.84022E-01	1.31361E+02	4.47637E-01	1.81118E+02	0.0	0.0	0.0	4.31747E+02
7	6.64122E-01	2.99138E+02	1.06395E+00	3.97761E+02	0.0	0.0	0.0	1.02534E+03
8	9.83770E-01	4.43020E+02	1.52775E+00	5.64583E+02	0.0	0.0	0.0	1.50848E+03
9	3.16205E-01	1.41285E+02	4.92591E-01	1.77438E+02	0.0	0.0	0.0	4.86750E+02
10	1.70571E+00	7.40227E+02	2.66928E+00	8.65115E+02	0.0	0.0	0.0	2.65510E+03
11	4.28151E+00	1.76890E+03	6.86480E+00	1.86248E+03	0.0	0.0	0.0	6.79624E+03
12	7.39636E+00	2.90382E+03	1.18191E+01	2.79108E+03	0.0	0.0	0.0	1.18213E+04
13	1.11170E+01	4.10943E+03	2.19359E+01	3.80838E+03	0.0	0.0	0.0	2.03648E+04

Fine-group edits like this are produced for each zone and for the entire system.

Each should be inspected to verify that the problem is well-converged. Generally one would expect the balance factors to be very close to 1.0 (±1%). In this case they are not, but the solution is still OK. See note on next page.

Because Zone 6 is the outermost zone, the RT BDY FLUX shown here should be the same as the scalar flux on the surface as later calculated by XSDOSE.

14	9.01372E+00	3.26642E+03	3.36875E+01	3.36571E+03	0.0	0.0	0.0	2.59935E+04
15	3.72606E+00	1.35046E+03	1.64275E+01	1.47523E+03	0.0	0.0	0.0	1.21364E+04
16	3.76067E+00	1.36157E+03	1.96563E+01	1.54105E+03	0.0	0.0	0.0	1.40625E+04
17	3.64851E+00	1.32265E+03	1.52368E+01	1.40488E+03	0.0	0.0	0.0	1.13876E+04
18	2.69873E+00	9.79732E+02	1.14612E+01	1.08756E+03	0.0	0.0	0.0	8.48182E+03
19	3.36508E+00	1.22425E+03	1.45822E+01	1.41838E+03	0.0	0.0	0.0	1.06916E+04
20	2.64416E+00	9.66219E+02	1.19426E+01	1.22310E+03	0.0	0.0	0.0	8.57981E+03
21	2.34853E+00	8.63759E+02	1.13293E+01	1.24261E+03	0.0	0.0	0.0	7.87924E+03
22	2.37674E+00	9.13756E+02	2.11324E+01	3.14790E+03	0.0	0.0	0.0	1.09579E+04
23	9.20293E+00	4.03186E+03	1.86977E+01	6.88227E+03	0.0	0.0	0.0	1.58447E+04
24	2.34978E+01	1.03302E+04	4.67363E+01	1.74068E+04	0.0	0.0	0.0	3.99850E+04
25	1.33958E+01	5.75875E+03	2.49460E+01	9.17257E+03	0.0	0.0	0.0	2.19315E+04
26	8.02271E+00	3.38108E+03	1.40570E+01	5.10588E+03	0.0	0.0	0.0	1.26979E+04
27	1.77433E+01	8.78618E+03	3.03164E+01	1.38611E+04	0.0	0.0	0.0	2.76694E+04
28	4.72354E+01	2.66682E+04	8.38847E+01	4.57668E+04	0.0	0.0	0.0	7.49792E+04
29	1.41567E+03	8.23360E+05	2.65797E+03	1.49777E+06	0.0	0.0	0.0	2.31302E+06
30	1.26565E+03	7.25868E+05	2.32635E+03	1.29649E+06	0.0	0.0	0.0	2.04365E+06
31	2.42931E+03	1.37202E+06	4.63636E+03	2.56333E+06	0.0	0.0	0.0	4.00433E+06
32	3.20407E+03	1.70229E+06	5.96146E+03	3.13736E+06	0.0	0.0	0.0	5.21133E+06
33	2.39796E+03	1.15946E+06	4.34551E+03	2.09930E+06	0.0	0.0	0.0	3.85828E+06
34	2.95427E+03	1.26259E+06	5.37380E+03	2.24158E+06	0.0	0.0	0.0	4.81266E+06
35	4.03742E+03	1.49192E+06	8.61054E+03	2.58859E+06	0.0	0.0	0.0	7.38404E+06
36	2.33064E+03	8.00636E+05	6.19299E+03	1.14827E+06	0.0	0.0	0.0	5.08958E+06
37	2.59214E+03	8.93326E+05	1.01467E+04	6.67588E+05	0.0	0.0	0.0	7.58010E+06
38	1.99169E+03	6.97218E+05	1.81568E+04	2.52671E+06	0.0	0.0	0.0	9.47848E+06
39	7.86355E+01	1.98757E+04	7.63247E+03	2.09222E+06	0.0	0.0	0.0	8.99214E+05
40	8.08495E-02	2.58020E+01	1.23739E+02	3.77389E+04	0.0	0.0	0.0	8.71851E+02
41	2.48770E+04	1.10305E+07	7.65832E+04	2.20208E+07	0.0	0.0	0.0	5.30245E+07

The Balance Factor shown on the previous page is defined as

$$BAL = 1 + \frac{\text{SOURCES} - \text{LOSSES}}{\text{SOURCES} + \text{LOSSES}} = \left(\frac{2S}{S+L}\right) \quad \text{where}$$

S = FIXED SOURCE + FISS SOURCE + IN SCATTER SOURCE + (N,2N) SOURCE

L = OUT SCATTER + ABSORPTION + NET LEAKAGE

$$\text{NET LEAKAGE} = \text{RT LEAKAGE} - \text{LFT LEAKAGE} = (\text{AREA})_{RB} \sum_m \mu_m w_m \psi_m \Big|_{RB} - (\text{AREA})_{LB} \sum_m \mu_m w_m \psi_m \Big|_{LB}$$

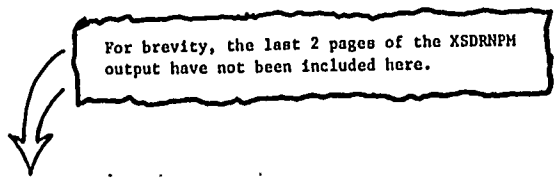
See additional comments on next page.

Regarding the strange balances shown on the previous two pages, several comments are in order:

1) Because of the way it is defined, group 1 will typically yield BAL=0.0 unless the zone contains some fissile material or a fixed volumetric source. Zone 6 contains neither.

2) As noted previously, the SCALE 22n-18Y cross section library properly accounts for the (n,2n) data in the 2-D transfer arrays, but the 1-D summary array for the (n,2n) data was dummied-out and set to zero. Since this term is all that is used to calculate the (n,2n) source rate shown here, the corresponding balance factors will be off for those first few high-energy neutron groups where the (n,2n) reaction is possible.

3) As noted previously, the SCALE 22n-18Y library contains the kerma factor in place of σ_A for the 18 gamma groups, so that $\phi\Sigma_A$ yields the energy deposition rate for groups 23-40 rather than the absorption rate. Thus, for this particular library, the balance factors printed for these energy groups will be meaningless. For other cross section libraries, however, they should be OK.



F4.5.5 XSDOSE OUTPUT WITH EXPLANATORY COMMENTS

```
**********************************************************************

PE CASK CONTAINING 15 2-YEAR-OLD PHR FUEL ASSEMBLIES

**********************************************************************

 IGE    =   2   SOURCE DISTRIBUTION (1/2/3/4 = SLAB/CYL/SPHERE/DISC)

  IP    = 100   NUMBER OF MESH INTERVALS IN PREVIOUS XSDRN CALC
 ISN    =  12   ORDER OF QUADRATURE USED IN PREVIOUS XSDRN CALC
 N16    =  16   UNIT ON WHICH ANGULAR FLUXES ARE TO BE READ
 N86    =  85   UNIT ON WHICH X-SECT DATA & DOSE FACTORS ARE TO BE READ
 MAST   =   0   DOSE FACTOR DATA ON A MASTER/WORKING LIBRARY (1/0)

  NG    =  22   NUMBER OF NEUTRON GROUPS (I.E. GROUPS  1  THRU  22)
  NI    =  18   NUMBER OF GAMMA GROUPS (I.E. GROUPS  23  THRU  40)

NDETEC=   4   NUMBER OF DETECTORS (I.E. PTS AT WHICH DOSE IS CALCULATED)
NFACTR=   2   NUMBER OF DOSE FACTOR ID NUMBERS TO BE ENTERED (SEE LIST)
NINCRM= 200   NUMBER OF INCREMENTS USED IN THE NUMERICAL INTEGRATION

DIMEN1= 9.90050E 01   RADIUS OF THE CYLINDER (MUST BE SAME AS XSDRN CALC)
DIMEN2= 5.08000E 02   HEIGHT OF THE CYLINDER (Z=0 TO Z=DIMEN2).
```

These two parameters will be read off the cross section library containing the dose factors; all the other parameters were specified by the user.

```
DOSE RATES AT THE VARIOUS DETECTOR POINTS WILL BE CALCULATED USING EACH
OF THE FOLLOWING SETS OF FLUX-TO-DOSE CONVERSION FACTORS (WHERE APPLICABLE):

MT=  9028    STRAKER-MORRISON CONVERSION FACTORS  (MREM/HR)/(NEUT/CM**2/SEC)
MT=  9501    STRAKER-MORRISON CONVERSION FACTORS  (MR/HR)/(GAMMA-RAY/CM**2/SEC)

NOTE: IF OUTPUT DOES NOT APPEAR FOR ANY OF THESE, IT IS BECAUSE THIS OR THAT
SET OF DOSE FACTOR DATA IS NOT AVAILABLE ON THE X-SECT TAPE SPECIFIED.
```

Because we wanted to enter 2 MT numbers, we set NFACTR=2 on the parameter card. Alternately, we could have entered a whole string of MT numbers and the code would have ignored those that it couldn't find.

	WEIGHTS	DIRECTIONS
1	0.0	-1.91151E-01
2	2.35877E-02	-1.35164E-01
3	2.35877E-02	1.35164E-01
4	0.0	-4.27285E-01
5	2.67348E-02	-3.94759E-01
6	2.67348E-02	-1.63514E-01
7	2.67348E-02	1.63515E-01
8	2.67348E-02	3.94759E-01
9	0.0	-6.38161E-01
10	2.66797E-02	-6.16416E-01
11	2.66797E-02	-4.51248E-01
12	2.66797E-02	-1.65167E-01
13	2.66797E-02	1.65169E-01
14	2.66797E-02	4.51248E-01
15	2.66797E-02	6.16417E-01
16	0.0	-8.09356E-01
17	2.53959E-02	-7.93805E-01
18	2.53959E-02	-6.72954E-01
19	2.53959E-02	-4.49654E-01
20	2.53959E-02	-1.57897E-01
21	2.53959E-02	1.57898E-01
22	2.53959E-02	4.49654E-01
23	2.53959E-02	6.72955E-01
24	2.53959E-02	7.93805E-01
25	0.0	-9.29892E-01
26	2.33492E-02	-9.18444E-01
27	2.33492E-02	-8.28540E-01
28	2.33492E-02	-6.57533E-01
29	2.33492E-02	-4.22161E-01
30	2.33492E-02	-1.45466E-01
31	2.33492E-02	1.45468E-01
32	2.33492E-02	4.22163E-01
33	2.33492E-02	6.57533E-01
34	2.33492E-02	8.28540E-01
35	2.33492E-02	9.18444E-01
36	0.0	-9.92127E-01
37	2.07622E-02	-9.83639E-01
38	2.07622E-02	-9.16605E-01
39	2.07622E-02	-7.87107E-01
40	2.07622E-02	-6.03968E-01
41	2.07622E-02	-3.79670E-01
42	2.07622E-02	-1.29497E-01
43	2.07622E-02	1.29499E-01
44	2.07622E-02	3.79671E-01
45	2.07622E-02	6.03969E-01
46	2.07622E-02	7.87108E-01
47	2.07622E-02	9.16606E-01
48	2.07622E-02	9.83640E-01

NOTE THAT THESE WEIGHTS AND DIRECTIONS MUST CORRESPOND TO THOSE OF THE PREVIOUS XSDRNPM CALCULATION

All these belong to "eta level number 4"

μ_m are listed in column labeled DIRECTIONS

$\eta_m = \sqrt{1.0 - \mu_{16}^2} = 0.344943 \quad m=16,\ldots,24$

Note that an S_{12} quadrature in cylindrical geometry has 48 discrete angular directions and that this quadrature set is identical with that used in the previous XSDRNPM calculation.

ANGULAR FLUX ON SURFACE OF CYLINDER

GROUP 1	(FLUX(IANGL), IANGL=1,NANGLS)						
0.0	0.0	3.71544E-04	0.0	0.0	0.0	3.53408E-04	1.51733E-03
0.0	0.0	0.0	0.0	2.34102E-04	1.68611E-03	4.90894E-03	0.0
0.0	0.0	0.0	0.0	1.01519E-04	1.27182E-03	5.26337E-03	1.19704E-02
0.0	0.0	0.0	0.0	0.0	0.0	-1.91744E-06	8.06418E-04
3.80997E-03	1.14702E-02	2.11724E-02	0.0	0.0	0.0	0.0	0.0
0.0	0.0	-5.72745E-05	4.56848E-04	2.40952E-03	7.56632E-03	1.79448E-02	2.78445E-02
GROUP 2	(FLUX(IANGL), IANGL=1,NANGLS)						
0.0	0.0	2.57986E-03	0.0	0.0	0.0	2.52198E-03	9.56441E-03
0.0	0.0	0.0	0.0	1.80118E-03	1.07087E-02	2.82493E-02	0.0
0.0	0.0	0.0	0.0	9.72458E-04	8.50592E-03	3.06019E-02	6.66801E-02
0.0	0.0	0.0	0.0	0.0	0.0	3.05951E-04	5.84422E-03
2.29805E-02	6.46391E-02	1.17208E-01	0.0	0.0	0.0	0.0	0.0
0.0	0.0	-7.14953E-05	3.71112E-03	1.53213E-02	4.37158E-02	1.00183E-01	1.54157E-01

- ✔ XSDOSE will edit the angular fluxes on the surface of the cask as calculated by XSDRNPM and stored on logical unit number N16.
- ✔ Groups 1-22 represent the neutron flux; groups 23-40 represent the gamma flux.
- ✔ Note: Of the 22 neutron groups, only groups 1 and 2 have any negative angular flux components. Obviously these are not physically real. See note on following page.

GROUP 21	(FLUX(IANGL), IANGL=1,NANGLS)						
0.0	0.0	2.90848E 00	0.0	0.0	0.0	3.02480E 00	4.10323E 00
0.0	0.0	0.0	0.0	3.00731E 00	4.36765E 00	5.19497E 00	0.0
0.0	0.0	0.0	0.0	2.94619E 00	4.35157E 00	5.48051E 00	6.18368E 00
0.0	0.0	0.0	0.0	0.0	0.0	2.86172E 00	4.21564E 00
5.37661E 00	6.38182E 00	6.94786E 00	0.0	0.0	0.0	0.0	0.0
0.0	0.0	2.76849E 00	4.01367E 00	5.07960E 00	6.12413E 00	6.92239E 00	7.38180E 00
GROUP 22	(FLUX(IANGL), IANGL=1,NANGLS)						
0.0	0.0	2.61024E 00	0.0	0.0	0.0	2.62861E 00	3.70723E 00
0.0	0.0	0.0	0.0	2.61689E 00	4.02859E 00	5.22059E 00	0.0
0.0	0.0	0.0	0.0	2.58119E 00	4.00272E 00	5.66885E 00	6.77686E 00
0.0	0.0	0.0	0.0	0.0	0.0	2.55668E 00	3.82659E 00
5.50993E 00	7.09264E 00	7.97569E 00	0.0	0.0	0.0	0.0	0.0
0.0	0.0	2.61349E 00	3.57957E 00	5.05437E 00	6.68421E 00	7.94329E 00	8.62998E 00

```
GROUP  23      (FLUX(IANGL), IANGL=1,NANGLS)

 0.0            0.0            2.37388E 00    0.0            0.0            0.0            2.56321E 00    1.76929E 01
 0.0            0.0            0.0            0.0            2.13573E 00    1.77096E 01    2.97169E 01    0.0
 0.0            0.0            0.0            0.0            1.85117E 00    1.22012E 01    3.31202E 01    3.24269E 01
 0.0            0.0            0.0            0.0            0.0            0.0            1.64333E 00    6.99691E 00
 2.99193E 01    3.53001E 01    3.35685E 01    0.0            0.0            0.0            0.0            0.0
 0.0            0.0            1.46188E 00    4.03932E 00    2.15118E 01    3.77383E 01    3.35324E 01    3.43237E 01

GROUP  24      (FLUX(IANGL), IANGL=1,NANGLS)

 0.0            0.0            6.21725E 00    0.0            0.0            0.0            6.69112E 00    4.37599E 01
 0.0            0.0            0.0            0.0            5.61082E 00    4.39971E 01    7.54695E 01    0.0
 0.0            0.0            0.0            0.0            4.80418E 00    3.05286E 01    8.36956E 01    8.39066E 01
 0.0            0.0            0.0            0.0            0.0            0.0            4.19009E 00    1.77336E 01
 7.50057E 01    9.09549E 01    8.76070E 01    0.0            0.0            0.0            0.0            0.0
 0.0            0.0            3.67931E 00    1.04113E 01    5.37217E 01    9.59415E 01    8.72875E 01    8.99234E 01
```

While not shown here, groups 28-32 each have several negative angular flux components. As noted previously, the use of a P_3 Legendre expansion to approximate the group-to-group angular scattering distribution(s) may give rise to negative angular fluxes in some energy groups. Typically they appear only in those directions (μ_3, μ_7, μ_{13}, μ_{21}, μ_{31}, μ_{43},.....) which are almost tangent to the surface of the cylinder (c.f. Fig. F4.2.14). Because of that, their small magnitude, and the infrequency with which they occur, they typically have no impact on the subsequent dose calculations. It is, however, something to be aware of. In this particular case (CYL: R=99.005 cm, 0≤Z≤508 cm), one should not try to calculate the dose at [R=99.010 cm, Z=5000 cm] unless he has performed the XSDRNPM calculation with a higher-order cross section set which enables him to accurately determine the angular flux component corresponding to μ_3.

```
GROUP  39      (FLUX(IANGL), IANGL=1,NANGLS)

 0.0            0.0            2.49927E 02    0.0            0.0            0.0            2.43462E 02    1.52343E 02
 0.0            0.0            0.0            0.0            2.42721E 02    1.38212E 02    1.14807E 02    0.0
 0.0            0.0            0.0            0.0            2.43812E 02    1.38079E 02    1.10202E 02    1.05114E 02
 0.0            0.0            0.0            0.0            0.0            0.0            2.45978E 02    1.43824E 02
 1.10863E 02    1.04151E 02    1.03362E 02    0.0            0.0            0.0            0.0            0.0
 0.0            0.0            2.49001E 02    1.54697E 02    1.14711E 02    1.04906E 02    1.03260E 02    1.03319E 02

GROUP  40      (FLUX(IANGL), IANGL=1,NANGLS)

 0.0            0.0            1.48790E-01    0.0            0.0            0.0            1.52036E-01    1.67473E-01
 0.0            0.0            0.0            0.0            1.52283E-01    1.67407E-01    1.66848E-01    0.0
 0.0            0.0            0.0            0.0            1.51540E-01    1.67401E-01    1.66513E-01    1.65657E-01
 0.0            0.0            0.0            0.0            0.0            0.0            1.50180E-01    1.67430E-01
 1.66585E-01    1.65330E-01    1.64480E-01    0.0            0.0            0.0            0.0            0.0
 0.0            0.0            1.48371E-01    1.67443E-01    1.66853E-01    1.65660E-01    1.64468E-01    1.63756E-01
```

FLUX AT DETECTOR 1

(R= 9.90050E 01, Z= 2.54000E 02)

GRP	SCALAR FLUX	
1	2.74955E-03	
2	1.56908E-02	
3	3.99559E-02	
4	1.35279E-01	
5	2.69098E-01	
6	2.84022E-01	
7	6.64122E-01	
8	9.83770E-01	
9	3.16205E-01	
10	1.70571E 00	
11	4.28151E 00	
12	7.39636E 00	
13	1.11170E 01	
14	9.01372E 00	
15	3.72606E 00	
16	3.76068E 00	
17	3.64851E 00	
18	2.69874E 00	
19	3.36509E 00	
20	2.64417E 00	
21	2.34853E 00	
22	2.37674E 00	
	6.07936E 01	(TOTAL NEUT FLUX)
23	9.20293E 00	
24	2.34979E 01	
25	1.33958E 01	
26	8.02271E 00	
27	1.77433E 01	
28	4.72354E 01	
29	1.41567E 03	
30	1.26565E 03	
31	2.42931E 03	
32	3.20407E 03	
33	2.39796E 03	
34	2.95427E 03	
35	4.03742E 03	
36	2.33064E 03	
37	2.59213E 03	
38	1.99169E 03	
39	7.86356E 01	
40	8.08496E-02	
	2.48166E 04	(TOTAL GAMMA FLUX)

Note: Detector 1 was intentionally located on the surface of the cylinder to demonstrate that the scalar fluxes calculated here by XSDOSE are identical with the right-hand boundary fluxes calculated by XSDRNPM. (See the fine-group summary printed by XSDRNPM for zone 6).

DETECTOR 1 (R= 9.90050E 01, Z= 2.54000E 02)

MT= 9028 STRAKER-MORRISON CONVERSION FACTORS (MREM/HR)/(NEUT/CM**2/SEC)

GRP	SCALAR FLUX	DOSE FACTOR	CALCULATED DOSE
1	2.74955E-03	2.08800E-01	5.74106E-04
2	1.56908E-02	1.65600E-01	2.59840E-03
3	3.99559E-02	1.47600E-01	5.89748E-03
4	1.35279E-01	1.47600E-01	1.99672E-02
5	2.69098E-01	1.40400E-01	3.77813E-02
6	2.84022E-01	1.33200E-01	3.78317E-02
7	6.64122E-01	1.29600E-01	8.60701E-02
8	9.83770E-01	1.26000E-01	1.23955E-01
9	3.16205E-01	1.26000E-01	3.98418E-02
10	1.70571E 00	1.29600E-01	2.21060E-01
11	4.28151E 00	1.33200E-01	5.70297E-01
12	7.39636E 00	1.18800E-01	8.78687E-01
13	1.11170E 01	5.40000E-02	6.00315E-01
14	9.01372E 00	6.48000E-03	5.84089E-02
15	3.72606E 00	4.32000E-03	1.60966E-02
16	3.76068E 00	4.68000E-03	1.76000E-02
17	3.64851E 00	4.68000E-03	1.70750E-02
18	2.69874E 00	4.50000E-03	1.21443E-02
19	3.36509E 00	4.32000E-03	1.45372E-02
20	2.64417E 00	4.14000E-03	1.09468E-02
21	2.34853E 00	3.96000E-03	9.30017E-03
22	2.37674E 00	3.78000E-03	8.98409E-03
			2.78996E 00 (TOTAL)

Total neutron dose at detector 1 (mrem/hr)

DETECTOR 1 (R= 9.90050E 01, Z= 2.54000E 02)

MT= 9501 STRAKER-MORRISON CONVERSION FACTORS (HR/HR)/(GAMMA-RAY/CM**2/SEC)

GRP	SCALAR FLUX	DOSE FACTOR	CALCULATED DOSE
23	9.20293E 00	9.79200E-03	9.01150E-02
24	2.34979E 01	8.28000E-03	1.94562E-01
25	1.33958E 01	6.84000E-03	9.16274E-02
26	8.02271E 00	5.76000E-03	4.62108E-02
27	1.77433E 01	4.75200E-03	8.43160E-02
28	4.72354E 01	3.96000E-03	1.87052E-01
29	1.41567E 03	3.49200E-03	4.94352E 00
30	1.26565E 03	2.98800E-03	3.78178E 00
31	2.42931E 03	2.41200E-03	5.85949E 00
32	3.20407E 03	1.90800E-03	6.11337E 00
33	2.39796E 03	1.60200E-03	3.84154E 00
34	2.95427E 03	1.26000E-03	3.72238E 00
35	4.03742E 03	9.21600E-04	3.72088E 00
36	2.33064E 03	6.37200E-04	1.48508E 00
37	2.59213E 03	4.39200E-04	1.13846E 00
38	1.99169E 03	2.37600E-04	4.73226E-01
39	7.86356E 01	1.40400E-04	1.10404E-02
40	8.08496E-02	3.02400E-04	2.44489E-05
			3.57846E 01 (TOTAL)

Total gamma dose at detector 1 (mr/hr)

FLUX AT DETECTOR 2

(R= 1.90445E 02, Z= 2.54000E 02)

GRP	SCALAR FLUX
1	1.31327E-03
2	7.43475E-03
3	1.86971E-02
4	6.23979E-02
5	1.20838E-01
6	1.24533E-01
7	2.84865E-01
8	4.20476E-01
9	1.34396E-01
10	7.07781E-01
11	1.70572E 00
12	2.83595E 00
13	4.09309E 00
14	3.28440E 00
15	1.35824E 00
16	1.36950E 00
17	1.33038E 00
18	9.85138E-01
19	1.23042E 00
20	9.70138E-01
21	8.66043E-01
22	9.06359E-01
	2.28225E 01 (TOTAL NEUT FLUX)
23	4.02648E 00
24	1.02957E 01
25	5.76773E 00
26	3.39631E 00
27	8.19847E 00
28	2.36184E 01
29	7.22206E 02
30	6.46774E 02
31	1.22762E 03
32	1.56196E 03
33	1.09514E 03
34	1.23135E 03
35	1.50197E 03
36	8.12407E 02
37	9.03057E 02
38	7.01182E 02
39	2.06593E 01
40	2.65104E-02
	1.04796E 04 (TOTAL GAMMA FLUX)

DETECTOR 2 (R= 1.90445E 02, Z= 2.54000E 02)

HT= 9028 STRAKER-MORRISON CONVERSION FACTORS (HREM/HR)/(NEUT/CM**2/SEC)

GRP	SCALAR FLUX	DOSE FACTOR	CALCULATED DOSE
1	1.31327E-03	2.08800E-01	2.74210E-04
2	7.43475E-03	1.65600E-01	1.23119E-03
3	1.86971E-02	1.47600E-01	2.75969E-03
4	6.23979E-02	1.47600E-01	9.20992E-03
5	1.20838E-01	1.40400E-01	1.69656E-02
6	1.24533E-01	1.33200E-01	1.65878E-02
7	2.84865E-01	1.29600E-01	3.69185E-02
8	4.20476E-01	1.26000E-01	5.29799E-02
9	1.34396E-01	1.26000E-01	1.69339E-02
10	7.07781E-01	1.29600E-01	9.17284E-02
11	1.70972E 00	1.33200E-01	2.27735E-01
12	2.83595E 00	1.18800E-01	3.36911E-01
13	4.09309E 00	5.40000E-02	2.21027E-01
14	3.28440E 00	6.48000E-03	2.12829E-02
15	1.35824E 00	4.32000E-03	5.86759E-03
16	1.36950E 00	4.68000E-03	6.41112E-03
17	1.33038E 00	4.68000E-03	6.22619E-03
18	9.85138E-01	4.50000E-03	4.43312E-03
19	1.23042E 00	4.32000E-03	5.31540E-03
20	9.70138E-01	4.14000E-03	4.01637E-03
21	8.66043E-01	3.96000E-03	3.42953E-03
22	9.06359E-01	3.78000E-03	3.42604E-03
			1.09167E 00 (TOTAL)

DETECTOR 2 (R= 1.90445E 02, Z= 2.54000E 02)

MT= 9501 STRAKER-MORRISON CONVERSION FACTORS (HR/HR)/(GAMMA-RAY/CM**2/SEC)

GRP	SCALAR FLUX	DOSE FACTOR	CALCULATED DOSE	
23	4.02648E 00	9.79200E-03	3.94273E-02	
24	1.02957E 01	8.28000E-03	8.52484E-02	
25	5.76773E 00	6.84000E-03	3.94512E-02	
26	3.39631E 00	5.76000E-03	1.95627E-02	
27	8.19847E 00	4.75200E-03	3.89591E-02	
28	2.36184E 01	3.96000E-03	9.35288E-02	
29	7.22206E 02	3.49200E-03	2.52194E 00	
30	6.46774E 02	2.98800E-03	1.93256E 00	
31	1.22762E 03	2.41200E-03	2.96102E 00	
32	1.56196E 03	1.90800E-03	2.98022E 00	
33	1.09514E 03	1.60200E-03	1.75441E 00	
34	1.23135E 03	1.26000E-03	1.55150E 00	
35	1.50197E 03	9.21600E-04	1.38421E 00	
36	8.12407E 02	6.37200E-04	5.17666E-01	
37	9.03057E 02	4.39200E-04	3.96622E-01	
38	7.01182E 02	2.37600E-04	1.66601E-01	
39	2.06593E 01	1.40400E-04	2.90056E-03	
40	2.65104E-02	3.02400E-04	8.01674E-06	
			1.64858E 01	(TOTAL)

For brevity, the results at detectors 3 and 4 may be summarized as follows:

DETECTOR 3 :	
NEUT FLUX = 1.20953(+1)	NEUT DOSE = 0.594526 mrem/hr
GAMMA FLUX = 5.90755(+3)	GAMMA DOSE = 9.681450 mr/hr
DETECTOR 4 :	
NEUT FLUX = 6.91587(+0)	NEUT DOSE = 0.332249 mrem/hr
GAMMA FLUX = 3.20909(+3)	GAMMA DOSE = 5.085330 mr/hr

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Computing Applications Division

COUPLE: SCALE SYSTEM MODULE TO PROCESS PROBLEM-DEPENDENT CROSS SECTIONS AND NEUTRON SPECTRAL DATA FOR ORIGEN-S ANALYSES

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ABSTRACT

The COUPLE code automatically couples problem-dependent cross-section constants and flux-weighting factors into libraries input to ORIGEN-S, for performing calculations of nuclear reactor isotope depletion and generation inventories and their associated sources and heat generation. In effect, the technique permits ORIGEN-S to apply multi-energy-group neutron cross-section data. The chief input required by COUPLE is simply a "Working Library" produced directly by the AMPX code system or the SCALE code system from neutronics analyses computed by BONAMI, NITAWL-II, and XSDRNPM.

Also, any of the nuclear data contained in ORIGEN-S binary libraries may be updated by the code.

The COUPLE code is one of the functional modules executed by the SAS2 control module of the SCALE code system. The source has been converted to FORTRAN 77 and implemented on the IBM 3090 and the CRAY X-MP mainframe computers and the IBM RS/6000 and the DEC ULTRIX workstation at ORNL.

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Many valuable suggestions concerning the code applications were received from users of COUPLE; those of most outstanding importance were provided by J. C. Ryman of the Computing Applications Division, J. R. Knight (retired from ORNL), and E. J. Allen (while with ORNL).

F6.1 INTRODUCTION

The function of the COUPLE code is the production of binary (unformatted) libraries to be input to the ORIGEN-S code, a program for computing concentrations of isotopes resulting from neutron irradiation or radioactive decay (reported in Sect. F7). One of the principal objectives in developing ORIGEN-S from the original ORIGEN code[1] was to extend the ORIGEN model to include multi-energy-group neutron flux and cross sections in any group structure. Further, it was desired that this function would be automated, in the respect that little or no user input data would be required. This objective is performed by COUPLE.

Three main functions may be applied by COUPLE:

1. An ORIGEN-S card-image library may be converted to a binary library, which saves computer time when input to ORIGEN-S and requires only two of the 35 library input data constants to be specified in the ORIGEN-S cases.
2. Any data in an ORIGEN-S binary library may be changed by using card input to COUPLE. These data not only include cross sections but all of the other nuclear data, such as decay constants, Q-values, effective branching fractions, spontaneous fission constants, and fission product yields.
3. Given any weighted AMPX library in the standard format of the SCALE system or AMPX system,[2,3] the entire set of neutron cross sections in an ORIGEN-S binary library may be updated to either one of the following: the reaction cross section included in the weighted AMPX library, as the priority option; or, the cross section computed from the old library few-group data and the improved flux-weight factors, updated from the AMPX library data. Note that data for a nuclide are included in a weighted AMPX library only when the nuclide is specified individually as part of the composition in describing the input to the code producing the library.

The primary significance of the procedures using COUPLE is that ORIGEN-S cross sections may be computed as a function of many of the design characteristics, operating parameters, and material compositions of a given nuclear reactor. Also, by changing the input composition at various times during a specified reactor irradiation history, several time-dependent libraries may be produced for input to a single ORIGEN-S case. A weighted AMPX library may be produced for user-specified systems by the BONAMI, NITAWL-II, and XSDRNPM modules (reported in Sects. F1, F2, and F3, respectively).

In general, the user follows the procedure described below. First, it is necessary that the user has available either the SCALE system master libraries, or the AMPX system master libraries, or the AMPX system (a modular code system for processing multigroup cross sections that is used frequently for criticality analyses). The evaluated and documented ENDF/B data base is processed to produce SCALE master libraries (reported in Sect. M4) which contain neutron cross sections in different group structures for a large number of nuclides. This type of library is produced similarly to an AMPX master library, except that the Nuclide Identification Number follows a certain convention for SCALE libraries. Next in the procedure the user processes a SCALE or AMPX master library through NITAWL-II (and/or BONAMI) and XSDRNPM for any reactor fuel-pin lattice to produce a weighted AMPX library required by COUPLE. Then a library is updated by COUPLE for input to ORIGEN-S, which computes irradiation and decay solutions to the reactor problem being analyzed. Variations to the procedure described above may be applied. The SAS2 (see Sect. S2) shielding analysis sequence provides an automated procedure similar to that described here. Irradiation-time-dependent compositions computed by ORIGEN-S may be used in subsequent cases by NITAWL-II and XSDRNPM, producing time-dependent ORIGEN-S libraries. Also, fuel-pin cells representing the compositions and temperatures in different zones of the reactor may be computed in order to more correctly "mock up," with different cell-weighted cross sections, the entire core of the reactor for producing more refined weighted AMPX libraries. In essence, once the user has produced the weighted AMPX library, which contains a set of cross-section constants that approximately apply to the specified problem, COUPLE will produce the updated library required by ORIGEN-S.

F6.2 ANALYTICAL METHODS APPLIED

Even though COUPLE is basically a data-management type of code, a few computational models are applied. The values of the three flux-weighting factors, named THERM, RES, and FAST in ORIGEN-S input, are computed for weighting cross-section group data of the large number of nuclides for which cross-section data are not included in the weighted AMPX library.

F6.2.1 FLUX-WEIGHT FACTORS

The convention used by the ORIGEN and ORIGEN-S codes is that the input flux be thermal flux and all cross sections be normalized to only the thermal flux. This section presents the model applied by COUPLE for deriving a set of library flux-weight factors that simulate the flux spectrum for the particular reactor lattice being analyzed. Where these factors are required for the large bulk of nuclides in ORIGEN-S libraries, the factors are not applied to the cross sections computed by XSDRNPM for the "composition" nuclides stored in the weighted AMPX library.

The effective cross section, σ_{eff}, should be derived from data in the initial ORIGEN-S libraries as a reasonable approximation to the definition:

$$\sigma_{eff} = \int_0^{\infty} \phi(E)\, \sigma(E)\, dE/\phi_{th}, \qquad \text{(F6.2.1)}$$

where

$$\phi_{th} = \int_0^{0.5\,eV} \phi(E)\, dE. \qquad \text{(F6.2.2)}$$

The approximation in ORIGEN and ORIGEN-S for σ_{eff} is

$$\sigma_{eff} = \text{THERM} \times \sigma_0 + \text{RES} \times I + \text{FAST} \times \sigma_1, \qquad \text{(F6.2.3)}$$

where

σ_0 = the 2200-m/s neutron absorption cross section,

$I = \int_{0.5\,eV}^{\infty} \frac{\sigma(E)}{E}\, dE$, the resonance integral,

σ_1 = the fission-spectrum-averaged cross section for all reactions with thresholds > 1 MeV.

Nuclide data not implicitly updated by COUPLE apply $\sigma_1 = 0$ for thresholds $\leq$1 MeV and both $\sigma_0 = 0$ and $I = 0$ for thresholds >1 MeV.

The flux-weight factors THERM, RES, and FAST applied by the codes are assumed to be constant for any specified reactor (or subcase). Obviously, since all nuclides do not have the same cross-section "distribution," Eq. (F6.2.1) cannot be derived from Eq. (F6.2.3) for all nuclides. Thus, idealized assumptions are applied in defining the flux-weight factors. Thermal reaction rates are assumed to follow that of a 1/v absorber, or

$$\sigma(E) = \frac{C_1}{v} = \frac{C_2}{\sqrt{E}} = \frac{\sigma_0\sqrt{E_0}}{\sqrt{E}} \qquad \text{(F6.2.4)}$$

$$\text{THERM} = \sqrt{E_0}\int_0^{0.5\,eV} \frac{\phi(E)}{\sqrt{E}}\, dE/\phi_{th}. \qquad \text{(F6.2.5)}$$

Using a Maxwell-Boltzmann distribution about T for the thermal neutron population, Westcott[4] derived

$$\text{THERM} = \sqrt{\frac{\pi}{4}\frac{T_0}{T}},\ T_0 = 293.16\ \text{K}, \qquad \text{(F6.2.6)}$$

where T is usually considered to be the absolute temperature of the reactor moderator. SCALE master libraries include a 1/v absorber material ($\sigma_0 = 1$), which may be included at a small density in the composition in the XSDRNPM case. When collapsed to the n groups of the thermal range, $\sigma(1/v)_{th}$, the broad group thermal value approaches the value of Eq. (F6.2.5) as $n \rightarrow \infty$,

$$\sigma(1/v)_{th} = \sum_{i=1}^{n} \phi_i\ \sigma(1/v)_i/\phi_{th}$$

$$= \sqrt{E_0}\int_0^{0.5\,eV} \frac{\phi(E)}{\sqrt{E}}\, dE/\phi_{th}, \qquad \text{(F6.2.7)}$$

or

$$\text{THERM} = \sigma(1/v)_{th} \qquad \text{(F6.2.8)}$$

is applied by COUPLE from the XSDRNPM calculation of $\sigma(1/v)_{th}$. Otherwise, T should be input to COUPLE and Eq. (F6.2.6) should be applied as an approximate alternative.

The standard computation of the resonance integral, I, implies a 1/E variation in the flux, which is a common assumption for, at least, approximating LWR flux. It has been shown (see Sect. F7.6.12) that RES can be derived from the 1/E assumption and the total resonance flux, ϕ_{res}. Thus,

$$\phi(E) = \frac{\phi_{res}}{\ell n(E_2/E_1)E}, \qquad \text{(F6.2.9)}$$

and from Eqs. (F6.2.1) and (F6.2.3),

$$\text{RES} \times \text{I} = \int_{0.5\,\text{eV}}^{\infty} \phi(\text{E})\, \sigma(\text{E})\, d\text{E}/\phi_{\text{th}}$$

$$= \int_{0.5\,\text{eV}}^{\infty} \frac{\phi_{\text{res}}}{\ell n(\text{E}_2/\text{E}_1)} \frac{\sigma(\text{E})}{\text{E}}\, d\text{E}/\phi_{\text{th}}$$

$$= \frac{\phi_{\text{res}} \text{I}}{\phi_{\text{th}} \ell n(\text{E}_2/\text{E}_1)}. \qquad \text{(F6.2.10)}$$

Thus, COUPLE computes RES from flux in the groups n+1 through m, inclusive (for the range 0.5 eV to 1 MeV) by applying

$$\text{RES} = \frac{\phi_{\text{res}}}{\phi_{\text{th}} \ell n(\text{E}_2/\text{E}_1)}$$

$$= \frac{\sum_{j=n+1}^{m} \phi_j}{\ell n(2 \times 10^6) \sum_{i=1}^{n} \phi_i}. \qquad \text{(F6.2.11)}$$

The factor FAST is applied only to the cross sections σ_1 for reactions with thresholds >1 MeV. It is assumed that ϕ(E) for E > 1 MeV is entirely from uncollided fission neutrons. Then, from Eqs. (F6.2.1) and (F6.2.3), and the fission spectrum flux, $\phi(\text{E})_f$:

$$\text{FAST} \times \sigma_1 = \int_{1\,\text{MeV}}^{\infty} \phi(\text{E})_f\, \sigma(\text{E})\, d\text{E}/\phi_{\text{th}}. \qquad \text{(F6.2.12)}$$

Also, by the definition of σ_1

$$\sigma_1 = \frac{\int_{1\,\text{MeV}}^{\infty} \phi(\text{E})_f\, \sigma(\text{E})\, d\text{E}}{\int_{\text{E}_f}^{\infty} \phi(\text{E})_f\, d\text{E}}, \qquad \text{(F6.2.13)}$$

where E_f is the lower bound of the fission spectrum flux $\phi(\text{E})_f$. Only a part of the fission neutron flux is above 1 MeV. The following ratio was computed:[1]

$$\frac{\int_{\text{E}_f}^{\infty} \phi(\text{E})_f\, d\text{E}}{\int_{1\,\text{MeV}}^{\infty} \phi(\text{E})_f\, d\text{E}} = 1.45 \qquad \text{(F6.2.14)}$$

Substituting Eqs. (F6.2.13) and (F6.2.14) into Eq. (F6.2.12),

$$\text{FAST} \times \sigma_1 = 1.45\ \sigma_1 \int_{1\,\text{MeV}}^{\infty} \phi(E)_f\, dE/\phi_{th}. \qquad \text{(F6.2.15)}$$

Thus, COUPLE computes FAST from the groups m+1 to k, inclusive (for the range 1 MeV to maximum energy) by applying:

$$\text{FAST} = \frac{1.45 \sum_{j=m+1}^{k} \phi_j}{\sum_{i=1}^{n} \phi_i}. \qquad \text{(F6.2.16)}$$

F6.2.2 CROSS SECTIONS COLLAPSED TO ORIGEN-S GROUP STRUCTURE

All nuclides in the weighted AMPX library (for which there is a nonzero ZA number) are more completely updated by COUPLE than those simply approximated with the flux-weight factors described above. The computed σ_{eff}, which ultimately is applied by ORIGEN-S, more nearly equals that of the definition in Eq. (F6.2.1). COUPLE computes σ_{eff} from the thermal flux groups 1 through n and all groups 1 through k, inclusive, by applying

$$\sigma_{eff} = \frac{\sum_{j=1}^{k} \phi_j \sigma_j}{\sum_{i=1}^{n} \phi_i}. \qquad \text{(F6.2.17)}$$

Note that Eq. (F6.2.17) retains the convention of ORIGEN for normalizing cross sections to thermal flux. The values produced by Eq. (F6.2.17) are stored in an ORIGEN-S working library.

A different algorithm is applied to data for an ORIGEN-S master library where three-group data are stored for a possible update by new flux-weight factors. Then the numerator of Eq. (F6.2.17) is reduced to include only the groups corresponding to those applied to the flux-weight factors. Also, the values computed are divided by THERM, RES, and FAST, respectively, in order that σ_{eff} will be correct once ORIGEN-S applies Eq. (F6.2.3), computing the subsequent products. While the procedure redundantly divides and later multiplies by the same value, it allows ORIGEN-S to use a consistent method for computing σ_{eff} properly by either Eq. (F6.2.3) or (F6.2.17) without requiring complex data management for the detection of which nuclides were updated by XSDRNPM. Also, by providing unweighted constants in the ORIGEN-S master library, the user may apply a more economical updating of fewer nuclides and use spectral shifts reflected in the three flux-weight factors for improving previously updated nuclides. The COUPLE edit of ORIGEN-S working libraries prints σ_{eff} as the total cross section plus the "unweighted" constants for the thermal, resonance, and fast energy groups.

The above model assumes that the SCALE or AMPX master library applies an energy group structure having a boundary at 0.5 eV and another at 1 MeV. When these boundaries are not in the energy group structure, COUPLE applies the nearest boundary. Even though this approximation does not alter the final value of σ_{eff} when Eq. (F6.2.17) is applied, it does affect those values updated from only the flux-weighting factors.

F6.2.3 THE APPLICATION OF MULTI-ENERGY-GROUP MODEL

Each energy group flux and cross section could be directly included in a nuclide depletion and generation model, in order to implement the multi-energy-group effect in the computation. However, it can be shown that this is not necessary.

The ORIGEN-S model solves the set of differential equations for the time rate of change of all nuclides. Each equation of the rate of change of a nuclide is simply the formation rate minus the removal rate of the nuclide. The equations solved by ORIGEN-S (see Sect. F7) have the following form, when expanded to explicitly apply G energy groups of ϕ and σ:

$$\frac{dN_i}{dt} = -(\lambda_i + \sum_{g=1}^{G} \sigma_i^g \phi^g) N_i + \lambda_{ji} N_j + \sum_{g=1}^{G} \sigma_{ki}^g \phi^g N_k + \ldots, \qquad \text{(F6.2.18)}$$

where

N_i = density or quantity of nuclide i
λ_i = decay constant of i
λ_{ji} = decay constant of nuclide transition j to i
σ_i^g = g^{th} group removal cross section of i
σ_{ki}^g = g^{th} group cross section of reaction k to i
ϕ^g = g^{th} group neutron flux

The + ... notation in Eq. (F6.2.18) indicates that other transitions to nuclide i are included. Then, denoting the effective cross section as σ^e and thermal flux as ϕ_{th} in Eq. (F6.2.18),

$$\sigma^e \phi_{th} = \sum_{g=1}^{G} \phi^g \sigma^g. \qquad \text{(F6.2.19)}$$

Substituting Eq. (F6.2.19) into Eq. (F6.2.18),

$$\dot{N}_i = -(\lambda_i + \sigma_i^e \phi_{th}) N_i + \lambda_{ji} N_j + \sigma_{ki}^e \phi_{th} N_k + \ldots. \qquad \text{(F6.2.20)}$$

This equation is identical to the equations solved by ORIGEN-S, which has the solution

$$\underset{\sim}{N} = \exp(\underset{\approx}{A}t)\, \underset{\sim}{N}(0), \qquad \text{(F6.2.21)}$$

where

$\underset{\sim}{N}$ = the vector nuclide quantities N_i

$\underset{\approx}{A}$ = transition matrix of constants in Eq. (F6.2.20)

$$a_{ii} = \lambda_i + \sigma_i^e \phi_{th} \text{ in } \underset{\approx}{A}$$

$$a_{ji} = \lambda_{ji} + \sigma_{ji}^e \phi_{th} \text{ in } \underset{\approx}{A}$$

Thus, the combination of using the neutronics codes, COUPLE and ORIGEN-S, implements the multienergy-group dependence of reaction rates into the model.

F6.2.4 DISCUSSION OF METHOD OF NORMALIZATION

The flux-weighting factors applied by ORIGEN and ORIGEN-S, as defined through Eqs. (F6.2.5), (F6.2.11), and (F6.2.16), are normalized to the thermal flux. This convention requires the one-group cross section, σ_{eff}, computed by Eq. (F6.2.17), to be normalized to thermal flux also. Since the more common convention is to normalize cross sections to total flux, the effect upon results from applying a different type of normalization appears to require a brief discussion. It is assumed that the values computed by Eqs. (F6.2.5), (F6.2.11), (F6.2.16), and (F6.2.17) are normalized consistently to any defined flux ϕ', where

$$\phi' = \text{constant} \times \phi_{th} = c\phi_{th}. \tag{F6.2.22}$$

Then when either the multigroup computation of Eq. (F6.2.17) or the ORIGEN-S process given by Eq. (F6.2.3) is applied, the value of any σ_{eff}, or σ, is changed to a value σ' as follows:

$$\sigma' = \sigma/c. \tag{F6.2.23}$$

The fission cross section, σ_f, becomes

$$\sigma_f' = \sigma_f/c, \tag{F6.2.24}$$

and similarly for all reaction cross sections. Consider cases in which specific power of the fuel is input to ORIGEN-S and the libraries contain σ' and σ'_f data. The flux ϕ that ORIGEN-S computes from σ_f data and the power, P, follows:

$$\phi = kP \Big/ \sum_i (\sigma_f)_i N_i, \tag{F6.2.25}$$

where k is dependent on energy per fission but independent of c. Throughout the computation of the ORIGEN-S solution (see Sect. F7.2), matrix elements applying cross sections always require the product $\sigma\phi$. We may examine the new product $\sigma'\phi'$ for the new normalization by, first, substituting Eq. (F6.2.24) into Eq. (F6.2.25) for ϕ',

$$\phi' = kP \Big/ \sum_i (\sigma_f')_i N_i$$

$$= ckP \Big/ \sum_i (\sigma_f)_i N_i$$

$$= c\,\phi \qquad \text{(F6.2.26)}$$

Thus, $\sigma'\phi'$ is simply the product of Eqs. (F6.2.23) and (F6.2.26):

$$\sigma'\,\phi' = \frac{\sigma}{c}(c\,\phi) = \sigma\,\phi\,. \qquad \text{(F6.2.27)}$$

This discussion proves that all matrix elements and the final computed concentrations do not change by applying c or a consistent change in normalization.

F6.3 PROGRAM STRUCTURE - SUBROUTINE FUNCTIONS

The COUPLE code is primarily a data-management program. Its main function is to provide a method of applying multigroup cross sections by the ORIGEN-S code. Data from a standard AMPX working library are coupled with an ORIGEN-S binary library to produce an updated library, containing the effective (single-valued) cross sections used by ORIGEN-S. Minimal card input data are required. Frequently all of the code default parameters are acceptable so that no card input of numerical data is required. Secondary functions of the code include converting a card-image library to a binary library and various updates of a library by card input. The code uses variable dimensioning and dynamical allocation of space. There are 76 subroutines (with approximately 6,000 source statements). The two subroutines that control the major flow paths in the code are SETUP and CNTROL.

F6.3.1 FLOW CHARTS

Figure F6.3.1 is a subroutine reference-type flow chart. It shows which subroutine calls each of the subroutines of the code. The larger blocks contain all of the "called" subroutines in alphabetical order to aid in locating any name. The code has two entry routines needed for application as either a "stand-alone" code or as a module called in by a SCALE control module. Control parameters for a case are initialized or read as input by SETUP. The various execution paths through the code, depending on the options requested, are controlled by CNTROL.

Figure F6.3.2 is a flow chart of the major paths of the code in the order in which the option decisions are made by CNTROL. Comments are given in parentheses, briefly stating the main function of subroutines. A block containing a comment represents a group of subroutines. These blocks are shown for updates of decay constants or cross sections from card-image data. The subroutines that are called for these updates are similar to those called for updating a library from an AMPX-produced library (starting at point "A" in the charts). The part from "A" to "B" performs variable dimensioning, reads and converts AMPX data, and reorganizes the data into a form that can be efficiently used in the final update treatment. The part starting at "B" shows the controlling flow for the updating process. The transition matrix and total capture cross-section data are separated into four separate arrays, three for the three energy groups and the other for decay data. The use of the "DO loop" allows the reading, processing, and writing of arrays for one group at a time. This procedure avoids storage-size problems and reduces computer time that results from using double dimensions and additional "DO loops." The matrix is compressed into a one-dimensional (1-D) array containing only nonzero transitions. Its size and structure (determined with a pointer array) is unchanged as long as new data contain only the same parent nuclides for any daughter nuclide (e.g., no new reaction types). Then the code may use the faster direct mode of updating with DIRECT. However, if the user requests the option, the matrix size and structure may be altered to contain any AMPX data for a new parent to a nuclide. This alteration is performed by NUMTRX.

Figure F6.3.3 shows most of the details in subroutine CHANGE, called from NUMTRX, for updating or adding new reaction data. This part is called when the user requests the addition of new parent nuclides. Broken lines indicate that other statements (i.e., updating capture data) have been omitted. The "DO loop to 40" is performed separately for each library receiving new data, where "library" refers to the light-element, actinide, and fission-product libraries. NN and N are the current pointers to the first nonzero element of "row I" of the old and new compressed matrix arrays, respectively, simulating the first parent having a transition to nuclide I. NN1 and N1 point to the first nondecay type transition element. The old data are first moved to the new arrays. Data are updated only when the next update nuclide, JDAUGH(KQ)=I. Then the old data are replaced if the parent J of I is found in the old array, or J=LOC(N2). If J is not already present, the row elements are expanded to include the new data. Nuclide ID numbers of update data (i.e., that from the AMPX library) were replaced in BYLOC with array pointers corresponding to I. The pointers to the update arrays given in the LP array were sorted by SORTP into the ascending order of I so that the complete update could be done in a single pass.

Names of called subroutines are listed alphabetically to aid in locating them.

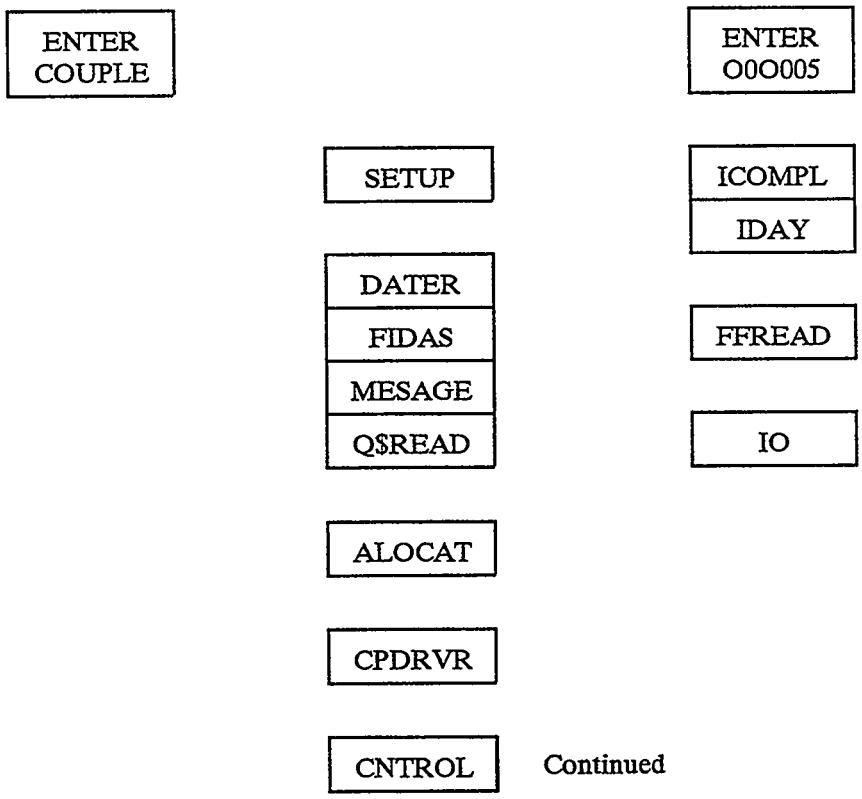


Figure F6.3.1. COUPLE code reference flow chart

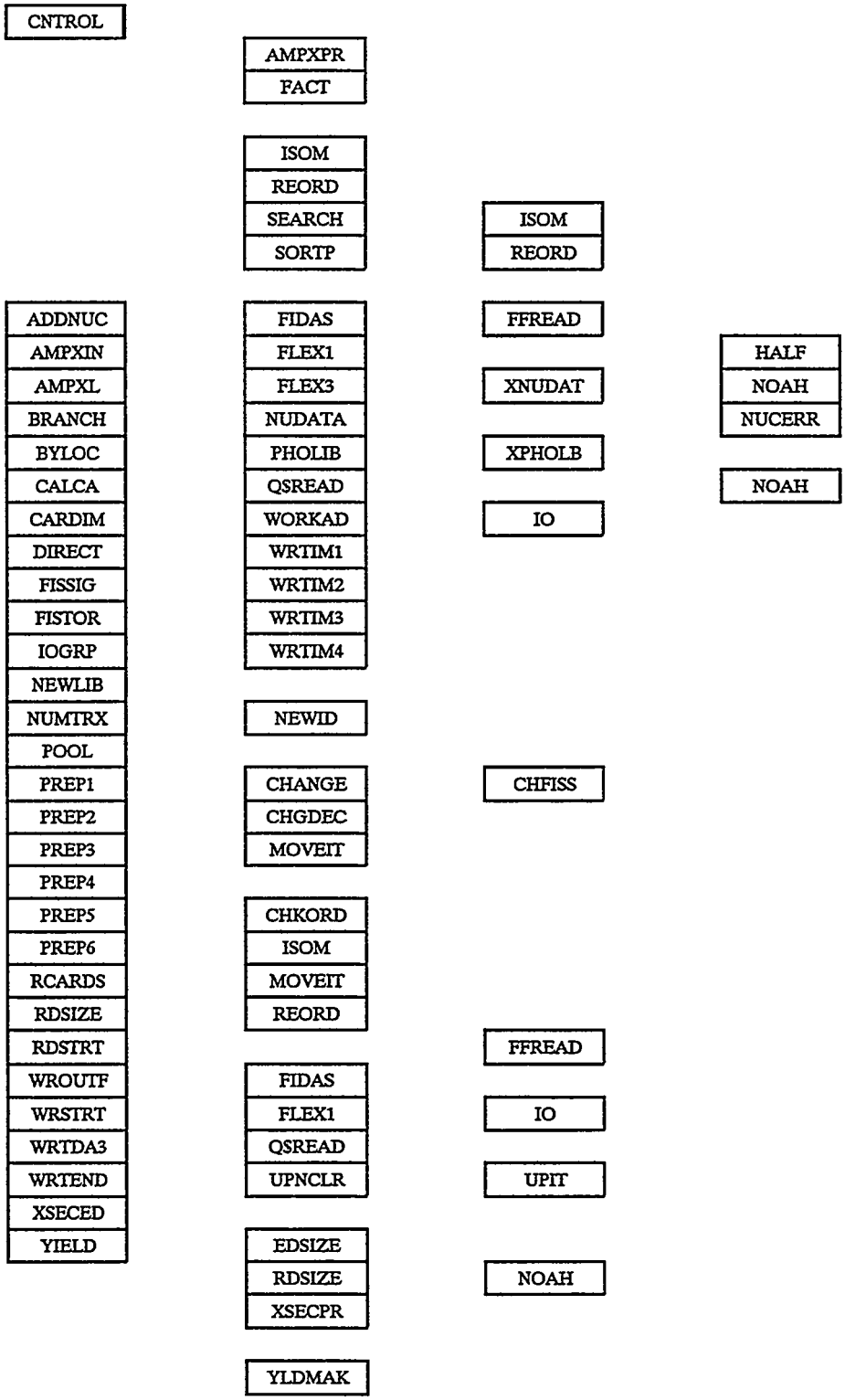


Figure F6.3.1 (continued)

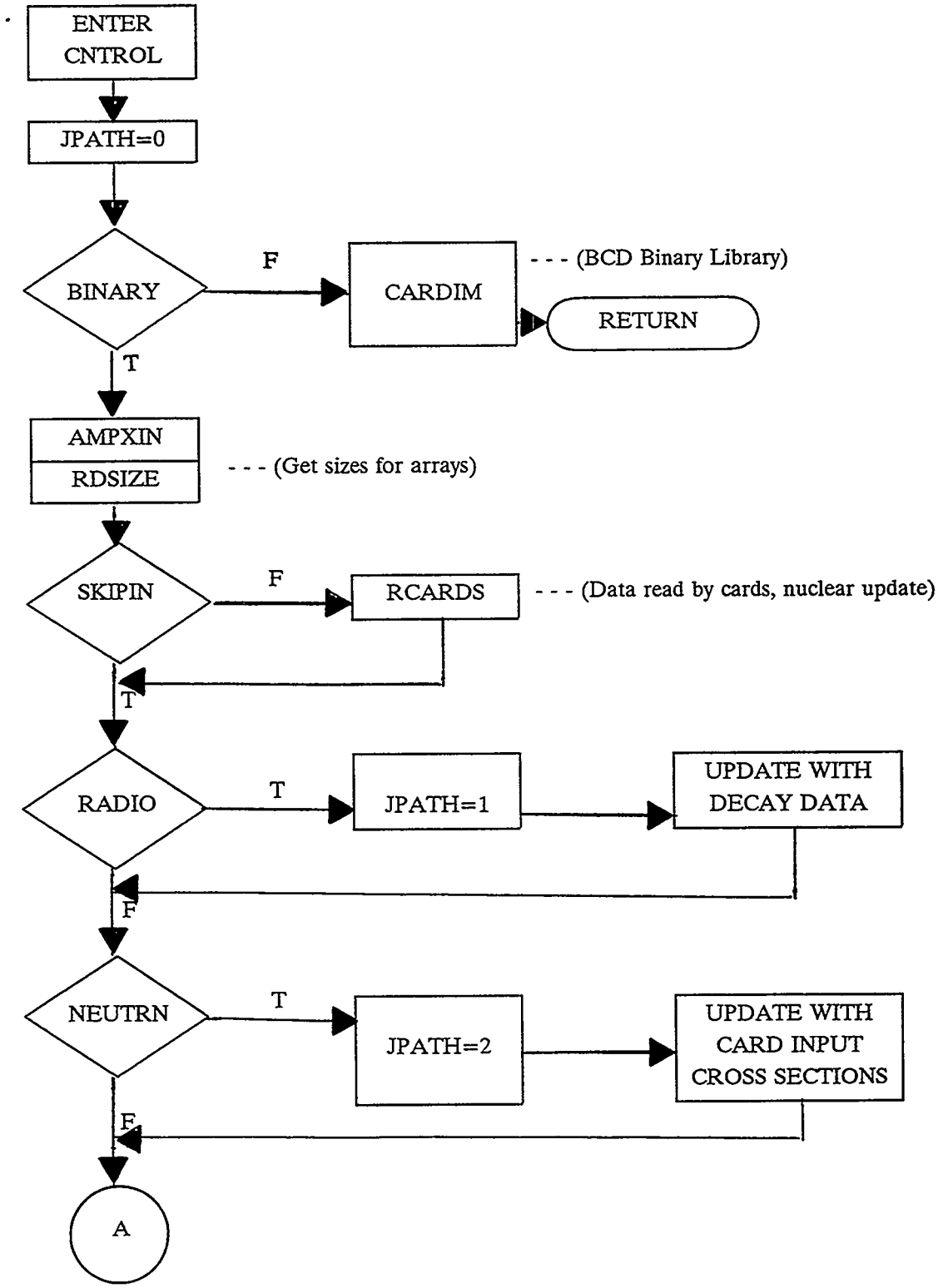


Figure F6.3.2 Flow chart of major paths

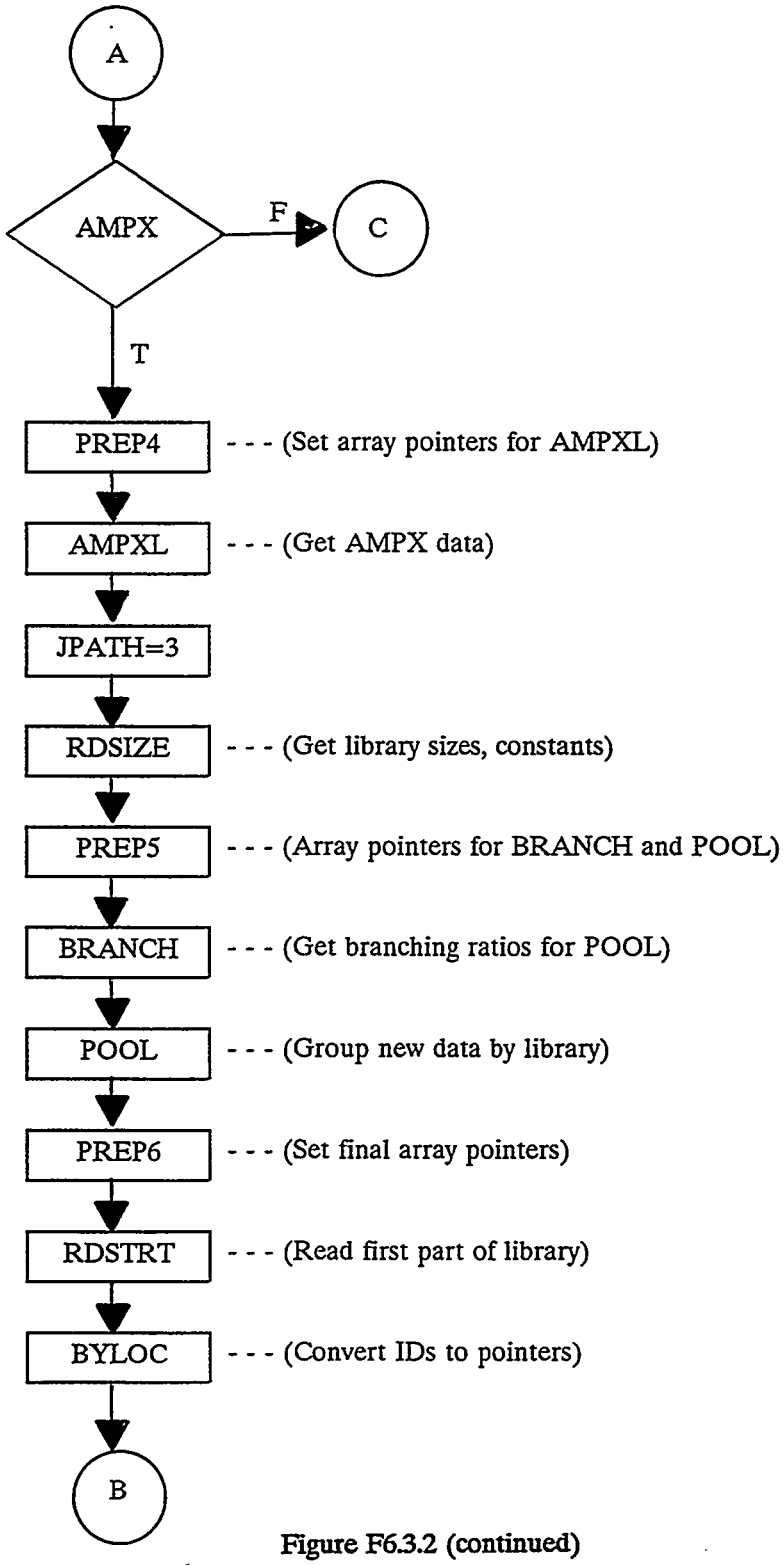


Figure F6.3.2 (continued)

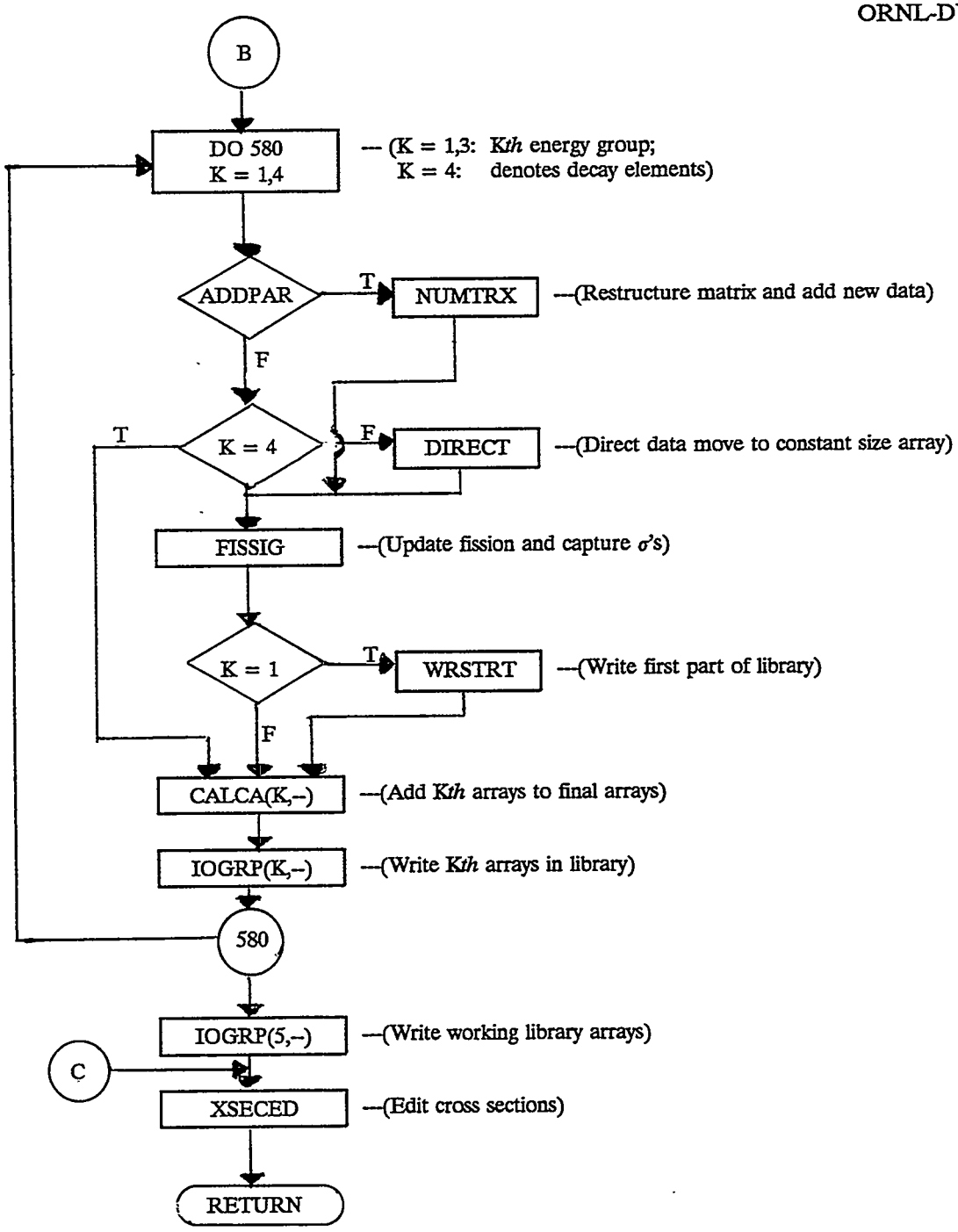


Figure F6.3.2 (continued)

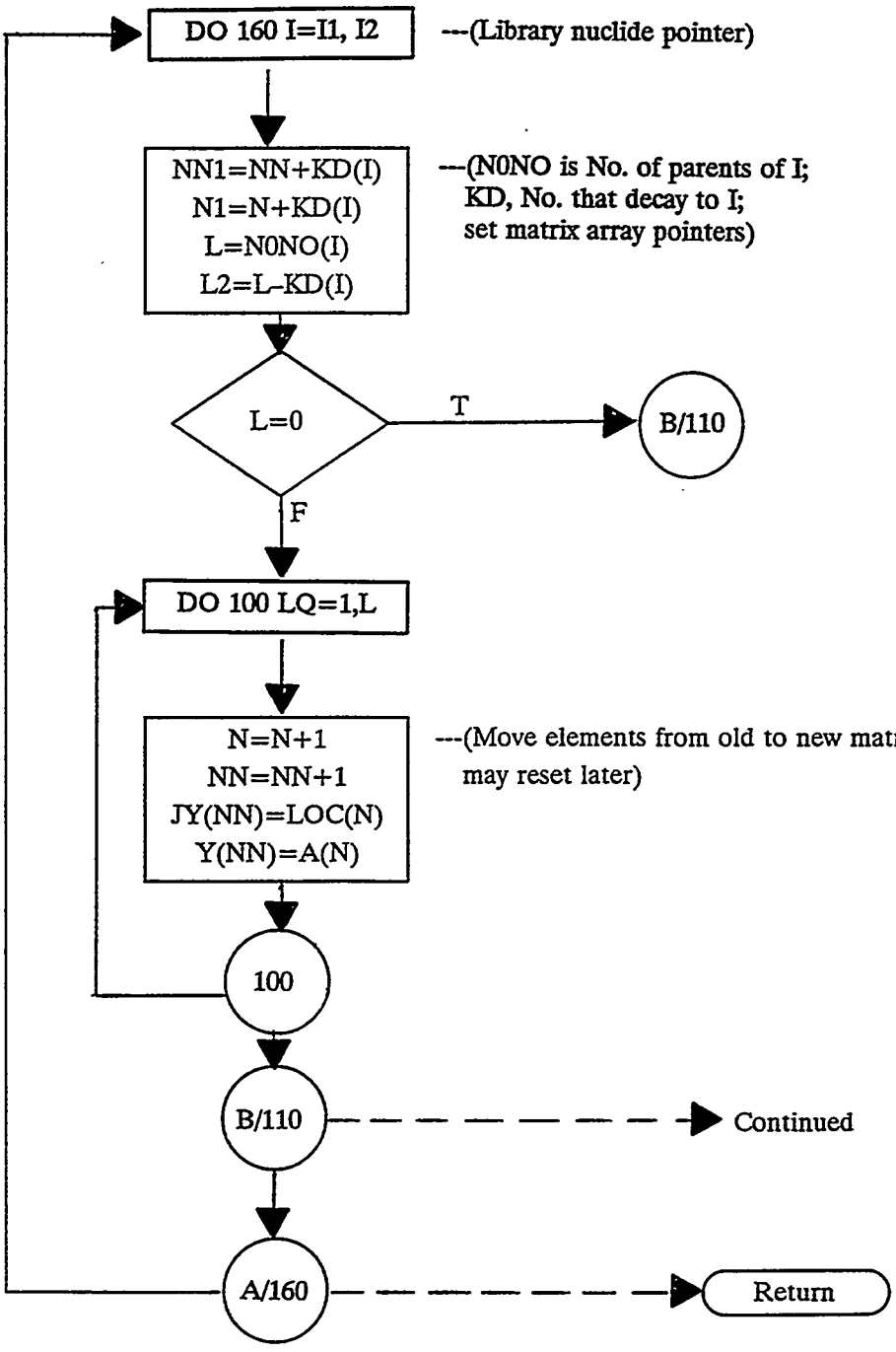


Figure F6.3.3 Flow chart for updating and adding reactions

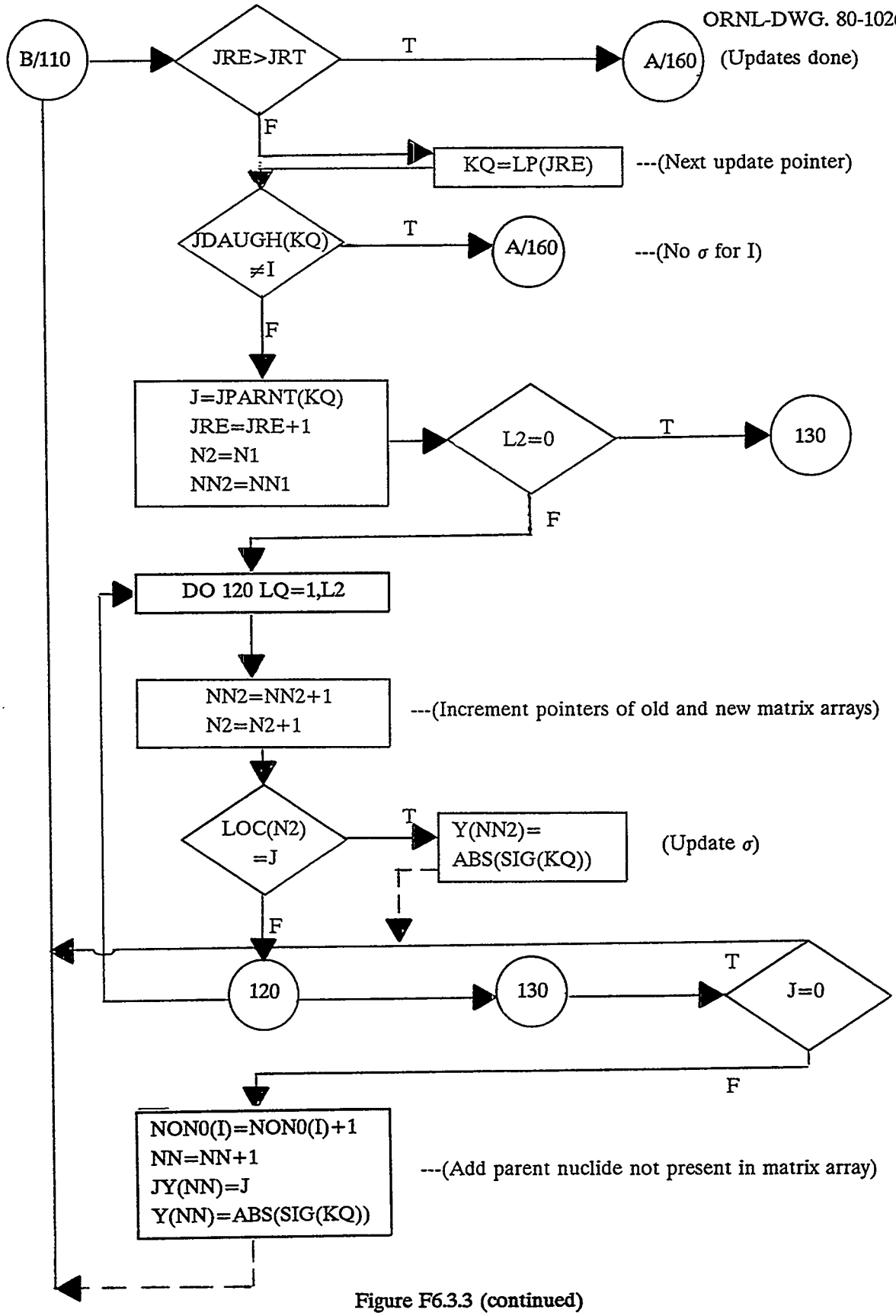


Figure F6.3.3 (continued)

(Note, on statement numbers shown on the flow charts: the code, as finally acquired by the user, may have statement numbers that differ from those given here because these may be changed in the normal external processing of source statements for SCALE system codes.)

F6.3.2 SUBROUTINE DESCRIPTION

Each subroutine is listed with a brief description of its fundamental purpose.

ADDNUC – Not used, at present.

ALOCAT – Allocates maximum space that can be allowed in the program's storage for the REGION size requested by computer job.

AMPXIN – Finds array sizes from the weighted AMPX working library.

AMPXL – Reads, normalizes and collapses XSDRNPM cross sections and determines daughter product nuclide ID numbers.

BRANCH – Since branching fractions are needed in using new (n,γ) and (n,2n) cross sections but are not given in binary library, the fractions are determined and stored for subroutine POOL.

BYLOC – Converts IDs of parents and daughters of new cross-section reactions to pointers to locations in ID array and sets pointers in an ascending order of daughter IDs.

CALC – Calculates final energy-dependent arrays, such as the transition matrix, using group-dependent array arguments and the weight factors of the group corresponding to each pass.

CARDIM – Controls the conversion of an ORIGEN-S card-image library to an ORIGEN-S binary library. Numerous array pointers are set and FIDO data blocks 3, 4, and 5 are read with calls to FIDAS. The card-image data are obtained in calls to NUDATA and PHOLIB. Individual energy group data are computed from arrays obtained with multiple calls to NUDATA in which the weight factors are set to either "1.0" or "2.0," as needed. A master library is written with four calls to WRTIMi (where i is 1, 2, 3, or 4). A working library is obtained with the additional call to WORKAD. Also, see Sects. F6.5.1, F6.5.2, F6.5.3, and F6.5.4.

CHANGE – Changes old cross sections (for energy group) to new XSDRNPM values and restructures the compressed transition matrix as needed.

CHFISS – Sets transition matrix elements used in producing fission products from a new fissile isotope, where the user specified that it be considered to have the same fission product yields as another fissile isotope.

CHGDEC – Same as subroutine CHANGE except that new decay transitions are changed or added.

CHKORD – Before subroutine POOL organized AMPX data, this routine checks nuclide ID numbers for ascending order. Some fission product libraries require the Z and A part of ID number to be reversed (temporarily for the code logic) to have ascending order.

CNTROL – Contains overall control of the major flow of the program. One or more calls to subroutines are made as a group, where each group performs a major function being requested (i.e., to update with AMPX data). These functions appear in the following order: convert card image to binary library, obtain updated values from card input, read library sizes, update half-lives, update with cross sections from card input, update with AMPX data, convert to ORIGEN working library and library cross-section edit.

COUPLE – An entry routine for "stand-alone" use of program (a MAIN, where NAME = COUPLE). It calls SETUP and ALOCAT.

CPDRVR – Called from ALOCAT to transfer a few data array pointers and call CNTROL.

DATER – Obtains date of execution of the job, for recording in new library and printed in completion statement.

DIRECT – Replaces transition values with updated area in the array SIG, when the new data require no additional elements in the transition matrix array.

EDSIZE – Edits the sizes of the 40 records (excluding first record) of the working library when cross-section edit is requested.

FACT – Computes the cross-section weighting factors, THERM, RES, and FAST, from the input reactor temperature or the 1/v absorber data and the flux spectrum produced by XSDRNPM-S code. The factors affect only the cross sections of nuclides not updated from the AMPX library.

FFREAD – Called from FIDAS for converting each FIDO card image data to operator characters, integers, or floating-point numbers, and returning the information in three arrays. It will permit either fixed-form or free-form input.

FIDAS – Uses data values and operators returned from FFREAD to determine all input arrays specified in a data block each time it is called. The input array numbers essentially point to the pointers of each array starting position in storage array.

FISSIG – Updates final fission and total capture cross-section arrays from data stored by POOL and AMPXL or read in by cards.

FISTOR – Moves (usually) updated fission cross section to SIGFID array for use by subroutine FISSIG. The cross sections may be unchanged for fission substitution, as obtained in subroutine POOL.

FLEX1, FLEX3 – Utility routines for moving arrays, or N words may be moved between areas located with starting pointers.

HALF – Converts half-life, in units designated, to a decay constant (in s^{-1}).

IO – Reads one record list of data from binary data set.

IOGRP – Writes (for K = 1,3) energy group-dependent arrays, A, TOCAP, FISS, and GENNEU in updated library data set. Reads the four records of arrays for next group. CNTROL sets K = 1, 5. Arrays A and DIS contain only decay transitions, if K = 4. The four final library arrays, composed by weighting group-dependent arrays with THERM, RES, and FAST, are written if K = 5.

ISOM – Makes right-hand digit = IT (an argument) in array NUX (or NUCL) for all ground state isomers, while adjusting other isomers of same nuclide (to IT + 1 or IT – 1) so that all ID numbers in NUX are in ascending order. Data management in code is enhanced by using ID-type arrays, or associated pointers, in an ascending order.

LABEL – A block data labeled common of chemical symbols of the elements.

INQOPN – If data set found to be unopened through an INQUIRE, calls OPNFIL (in SCALE library) to open it.

MOVEIT – Moves transition matrix data from old to updated array for any of the three libraries, if nothing is to be updated in the library.

MULTN – Computes the neutron production array, GNU (for changing GENNEU), of light-element and actinide nuclides for which the (n,2n) and (n,3n) reactions are updated.

NEWIO – Converts working to master library (or reverse) if requested by NEWID. Checks for new weight factors in FAC array and uses them for THERM, RES, and FAST. If zero, uses those from input library.

NEWLIB – Sets array pointers for call to subroutine NEWIO.

NOAH – Converts nuclide ID to isotopic chemical symbol.

NUCERR – Writes error message when called from XNUDAT.

NUDATA – An interface, which calls XNUDAT with proper pointers as element to the storage array, in providing flexible dimensioning.

NUMTRX – Controls the calls and arguments needed for subroutines that update cross sections and restructure the compressed transition matrix.

PAGE – Writes a page giving references to card-image library data, if converting to binary library. However, this edit has not been implemented.

PHOLIB – An interface, which calls XPHOLB with proper pointers as element to the storage array, in providing flexible dimensioning.

POOL – Reorganizes new cross-section data from AMPXL or RCARDS so that library data are grouped together, reactions where parent or daughter is not in library are deleted, and certain flags are made (using negative sigmas or IDs) for fissile or by-product nuclides.

PREP1, 2,3,4,5, and 6 – With the exceptions of CARDIM, XSECED, UPNCLR, YIELD, and RCARDS, these subroutines perform all the flexible dimensioning and allowable overlaying of storage for the COUPLE code. Each PREPi, where i = 1, 6, prepares arrays for functions, i, as follows:

1. adding nuclides from cards to library (not implemented),
2. master library decay update,
3. master library neutron reaction update,
4. obtaining AMPX data from AMPXL,
5. reorganizing AMPX data in BRANCH and POOL, and
6. completing working library update with AMPX data.

Q$READ – Reads input case data from binary interface data set produced by a SCALE control module.

O0O005 – Entry routine used only when called from a SCALE system control module. Data will be read on a binary interface data set.

RCARDS – Reads FIDO input card data to be used for updating master library, flexibly dimensioning arrays needed for storing of data.

RDSIZE – Reads current input binary library first record to obtain all array sizes and other constants in that library, and stores them in COMMON/SIZES/ and /PARMS/.

RDSTRT – Reads start of binary library, or records 2-12 inclusive. This sets all arrays stored from library through first energy group of A, TOCAP, FISS, and GENNUE.

REORD – Reverses the Z and A parts of the nuclide ID number when found necessary by CHKORD to make ascending order.

SEARCH – Checks library to determine if both parent and daughter are present, applying table-splitting method.

SETUP – Sets defaults and reads input of primary control parameters and unit numbers. Opens all data sets used and writes message if undefined unit is needed. Execution of each case starts and ends in the routine.

SORTP – Sorts an integer array (NUCL, JDAUGH, etc.) into ascending order and makes some rearrangement to the pointer array associated with the array.

UPIT – Edits old and new data in "nuclear data update" as set up by subroutine UPNCLR.

UPNCLR – Updates card input "nuclear data" [nontransition data (i.e., Q values, abundances, and photon spectra)]. See input description of Data Block 7.

WI, WJ – Debug print routines, retained because they remain useful. Writes 8-character word (usually variable name) and a specified number of words, integers, or floating point, starting with a specified variable (i.e., the variable for which name was printed).

WORKAD – Adds the part of working binary ORIGEN-S library needed to change master to working library. Used when converting card-image library to binary working library.

WROUTF – Edit routine not implemented.

WRSTRT – Writes first eight records of updated binary library, through array LOC.

WRTEND – Copies records 27 through 40 (end) from input to output binary library.

WRTIM1, 2, 3, and 4 – Writes the records, each (except first two) containing a single array, that are developed in converting the card-image library to a binary library. They print out the start and end of each array.

XNUDAT – This is almost the same as XNUDAT in ORIGEN-S code. Reads card-image nuclear library, processing data with three weight factors into needed arrays.

XPHOLB – Almost same as XPHOLB in ORIGEN-S code. Reads card-image photon libraries.

XSECED – Makes flexibly dimensioned arrays needed for XSECPR and edits titles and weight factors.

XSECPR – Reads binary library cross sections and prints out total for each reaction and the unweighted group values for the reaction, removal, and fission cross sections.

YIELD – Sets array pointers for call to YLDMAK.

YLDMAK – Makes temporary library where fission product partial sigma group values, if zero, are changed to the fission-product yield fraction times the minimum machine word size (XLOW) divided by the minimum yield fraction of all fission products (YLDMIN). This feature allows update from a fission cross-section group value that is zero to a nonzero value.

F6.4 FEATURES AVAILABLE AND PROCEDURES

The main objective of the COUPLE code is the implementation of the effective application of multigroup cross sections in ORIGEN-S. Even though all options and features of the code are given in the input description (Sect. F6.5), this section presents additional discussion pertaining to the purposes of these features. The reader may want to read at least the introductory section and the definition of libraries (Sect. F6.5.1) before reading this.

F6.4.1 CONVERTING TO BINARY LIBRARY AND GENERAL FEATURES

The various features include:

1. Any ORIGEN-S or ORIGEN (formatted) card-image library for the reactor type specified by the flux-weighting factors may be converted to an ORIGEN-S binary library.

2. A library ID number may be input by the user and stored in the library for identification purposes.

3. Either an ORIGEN-S master binary library or an ORIGEN-S working library may be produced by selection of a proper library ID number.

4. The same library constants and size parameters that are specified in ORIGEN-S input for card-image libraries are required in a similar manner in COUPLE input. However, when using the binary library later, by either code, these input data are not required.

5. An ORIGEN-S master library may be converted to an ORIGEN-S working library by specifying the proper options, the library ID number, and the flux-weighting factors.

6. Up to 40 title cards may be contained in a library. These are printed in ORIGEN-S cases. When updating binary libraries, the user may specify the number to keep (starting with the first card) and may input additional title cards which, in the new library, precede those that were kept.

7. Multiple options are available and stacked cases within one job are permitted. However, the user should be warned that some combinations of options may not be well tested and, when in doubt, stacking cases is the normal method. For example, when converting to a binary library or updating a library, a library edit is normally requested in a short stacked case. Also, updating options should follow in a separate case after converting to a binary library.

8. Useful edits are available. During an "updating" case, all new values are edited. Also, a complete edit of reaction, fission, and removal cross sections of any binary library may be requested. Although other nuclear data may not be edited by COUPLE, these data, as contained in the card-image libraries, may be edited by ORIGEN-S. The binary library format is presented in Sect. M6.

F6.4.2 COMPUTED CROSS-SECTION UPDATING

Updating ORIGEN-S binary libraries from a weighted AMPX library has the following features:

1. The above option is the default. When all other defaults apply, the updated ORIGEN-S working library may be produced simply from card input consisting of a blank card (to "end" the title), followed by the required "DONE" card and using defaulted unit numbers in the job control language.

2. When the weighted AMPX library multigroup cross sections are not collapsed to the ORIGEN-S energy group structure, the collapse may be performed by COUPLE.

3. The thermal flux-weighting factor, THERM, will be computed by COUPLE when the user includes the "1/v absorber material" as a small density in the fuel zone composition "mixing table" of the XSDRNPM-S case that produces the weighted AMPX library; or THERM may be computed through the input of the average moderator temperature. The former model is applied when the 1/v absorber data are included in the weighted AMPX library. Normally, it is more accurate than the computation using temperature.

4. An option is available for adding new precursor transitions to the ORIGEN-S working library for all reactions for which there are data in the weighted AMPX library, provided both the target and product nuclides are included in the ORIGEN-S working library. (See Sect. F6.5.5 for further details.)

5. The user may specify the nuclide ID number of the nuclide data from which the flux data are used to compute the flux-weighting factors. For the default, the code applies the same nuclide as given in the input ORIGEN-S library, or, if it is zero, the flux data for the first nuclide in the weighted AMPX library are applied. When applying "region weighting" in the XSDRNPM-S case, the user should be warned that the last default could produce incorrect flux-weighting factors, if the first nuclide is contained in the moderator or clad material. Note that all nuclides in the fuel zone only have the same flux distribution, producing the same flux-weight factors.

6. As an approximation, the user may substitute the fission yield data of one fissile isotope for that of another fissile isotope having no data. Although not always desirable, this substitution may improve results or eliminate nonconservative results.

7. The user may choose between producing cell-weighted, zone-weighted, or region-weighted cross sections as an option in the XSDRNPM-S case. The type of weighting that should be selected depends upon the user's objective. As an example, consider a case in which a fuel-pin lattice is being analyzed with a single material zone for each of the three materials: fuel, clad, and moderator. The weighting model is a function of the flux spectra, number densities, and volume fractions of the zones. Cell weighting produces cross sections that represent the "mock-up" of the fuel-pin cell as a single homogeneous region. Zone weighting produces data for each zone separately, such that different cross sections are computed for each zone in which a nuclide is present. Region weighting computes only a single set of data per nuclide, but applies only the flux from the regions containing the nuclide. Zone weighting is not permitted by COUPLE (without applying special utility code processing of the libraries),* since the weighting procedure may produce more than one set of data for a single nuclide and uncertain COUPLE results. The following discussion applies mainly to LWRs, and, in particular, to PWRs instead of other designs such as LMFBRs.

   The question may arise as to the differences in concentrations computed by ORIGEN-S caused by applying cell or region weighting. Consider that there are four classes of nuclides:

   1. nuclides contained only in the fuel zone and updated in the weighted AMPX library,

   2. other fuel zone nuclides present in the ORIGEN-S library,

   3. nuclides contained in the nonfuel zone and updated in the weighted AMPX library, and

*The FIXZA code was written for this purpose.

4. all other nuclides in the ORIGEN-S library not in the first three classes.

The cross sections of all nuclides of the first class change by the same constant when converting from region-weighted values to cell-weighted values. Thus, when applying the same power in ORIGEN-S cases, the reaction rates and subsequent concentration results of these nuclides are not changed (see Sect. F6.2.4). Also, when a flux consistent with the type of weighting is input to ORIGEN-S, the results of these nuclides remain unchanged.

The fuel zone nuclides of class 2 are computed by Eq. (F6.2.3) and the updated flux-weight factors. When THERM is determined from $\sigma(1/v)_{th}$, it is changed by the same constant as the other cross sections in converting to cell weighting. However, the effective conversion constants for RES and FAST are different from that applied to THERM. Let ϕ_{th}, ϕ_r, and ϕ_f represent the group flux values of the fuel zone for the thermal, resonance, and fast neutron energies, respectively, and superscript "c" refer to cell values. The following equations are derived from preserving reaction rates in the weighting option:

$$F = \frac{THERM^c}{THERM} = \frac{\phi_{th}}{\phi_{th}^c} \qquad \text{(F6.4.1)}$$

$$\frac{RES^c}{RES} = \frac{F\phi_r^c}{\phi_r} \qquad \text{(F6.4.2)}$$

$$\frac{FAST^c}{FAST} = \frac{F\phi_f^c}{\phi_f} \qquad \text{(F6.4.3)}$$

Computations by XSDRNPM-S for PWR lattices indicate that ϕ_r^c/ϕ_r is usually in the range 0.99 to 1.00 and ϕ_f^c/ϕ_f varies between 0.96 and 0.98. THERM [computed from $\sigma(1/v)_{th}$] is calculated in the same manner as cross sections of nuclides in class 1. Since THERM, RES and FAST are, at best, computed as a reasonable approximation to a more rigorous model, the differences in final results due to weighting option for the nuclides in class 2 appear to have small relative significance.

The differences between cell and region weighting may produce a change in concentrations computed by ORIGEN-S for the nonfuel zone nuclides of class 3. Cross sections computed by COUPLE are determined correctly for either the cell-weighted or zone-averaged flux applied. However, when power is input to ORIGEN-S, the thermal flux of the fuel zone is computed and then applied to all nuclides. Since it is observed from PWR lattice computations that the thermal flux of the fuel is usually about 0.90 to 0.95 times that of other zones, these factors proportionately affect the reaction rates of the light elements computed from applying region weighting. The ORIGEN-S case would require the input of the proper zone flux for the concentrations of these nuclides to be correctly computed.

The nuclides of class 4 include light elements that are not updated. As in the case of class 2, the cross sections applied are a function of THERM, RES, and FAST. Normally, the user specifies that these factors be computed from the flux pertaining to one of the fuel nuclides. Thus, with either type of weighting option, results calculated for nuclides of class 4 reflect this inconsistency. Additionally, the differences given above for nuclides in class 3 apply similarly to class 4.

A few primary conclusions may be derived from the above discussion. Cell weighting, when generally applied to updating all types of nuclides, appears to produce more consistent or correct

results in ORIGEN-S cases than those produced from the region weighting option. However, when the objective is mainly the updating and computation of fuel and fission-product nuclides, with no calculations required for light elements, there are essentially minor, or no, differences in the results of the important nuclides due to the selection of type of weighting. Since most of the cross sections in the card-image library of ORIGEN-S and ORIGEN were taken from student references such as BNL-325, except for those computed from a fuel-pin lattice cell calculation, these are zone-weighted cross sections according to the above definitions.

8. The LMFBR type of library may be updated properly with COUPLE. The card-image library for the LMFBR applies a difference rule: THERM, RES, and FAST are set to "1.0." COUPLE maintains this rule. Cross sections that are updated in producing the weighted AMPX library are updated in the ORIGEN-S binary library, while all others remain unchanged.

F6.4.3 OTHER NUCLEAR DATA UPDATING

The updating capability of COUPLE is complete, in the respect that any data or value in any ORIGEN-S binary library may be changed through the use of card input (see Data Blocks 6–9 of input description, Sect. F6.5). These features are briefly presented in the following:

1. Any nontransition "nuclear data" may be updated. These data are defined with their "code variable names:"
   - DIS – Total decay constant.
   - Q – Total decay energy released (MeV).
   - FG – Fraction of energy Q from photon emission.
   - AMPC – Radioactive concentration inhalation guide value, RCG_a.
   - WMPC – Radioactive concentration ingestion guide value, RCG_w.
   - ABUND – Atom percent abundance of a naturally occurring isotope.

2. Photons/disintegration spectra of any nuclide in the photon energy group structure of the library may be updated. (However, a more automatic update from the master photon library is done by ORIGEN-S.)

3. Neutron reaction cross sections of any nuclide for any transition may be updated by card input. Any neutron reaction is permitted, since the type of reaction is simply denoted by input of the target and product nuclides. Also, nonfission removal and fission cross sections may be updated by card input.

4. Fission yield data may be updated indirectly by using the yield fraction of the fission product times the fission cross section of the fissile nuclide as an updated transition. (A separate updating code may be more efficient for processing a complete update of fission yields.)

5. The user may substitute the fission yield data of one fissile isotope for that of another which has no yield data. Even though these yield data may not be correct, it may be an improvement over the alternative that effectively means all yields are zero for the isotope; and the substitution may, at least, produce more conservative results. This option may be requested when updating by card input here or in the "computed cross-section updating" using a weighted AMPX library.

6. Decay constants and branching fractions may be updated. The product of branching fraction and proper decay constant is simply input for the proper transition between two nuclides to produce the branching fraction updating.

F6.5 COUPLE CODE INPUT DESCRIPTION

The COUPLE code is used in conjunction with the ORIGEN-S code and other codes in the SCALE and AMPX systems. Its principal purpose is to implement, with minimal effort on the part of the user, the effective use of multigroup cross sections in subsequent burnup and decay computations by the ORIGEN-S code. The cross sections are usually produced by executing the XSDRNPM-S code for a case that represents the reactor conditions under consideration (i.e., lattice geometry and time-dependent densities).

Even though the card input data needed to couple AMPX cross sections into an ORIGEN-S library are usually only a few entries (since defaults readily apply), the input description encompasses many methods of updating the wide variety of other data contained in ORIGEN-S libraries. When pursuing efforts to enhance greater accuracy, the user may need to "correct" or "improve" some of the other data through these methods.

General comments and definitions are presented first. Also, prior reading of the sections on "Introduction to COUPLE" and "Features Available and Procedures" is suggested.

F6.5.1 DEFINITION OF LIBRARIES

The main function of the code is converting or updating of libraries (also, see "ORIGEN-S Data Libraries," Sect. M6). The different types of libraries are defined as follows:

1. ORIGEN-S Card-Image Library
   This library is any formatted (BCD) nuclear data library that can be used by ORIGEN-S. When its data are acceptable, it may be used directly for ORIGEN-S cases. Only a part of it is updated when using the COUPLE code.

2. ORIGEN-S Binary Library
   This library is the type of library obtained when either converting an ORIGEN-S library to binary mode or updating another binary library. It can have two different record structures as given in the two following definitions.

3. ORIGEN-S Master Library
   This library is an ORIGEN-S binary library containing originally all of the data, including three-group (unweighted) cross sections, of an ORIGEN-S card-image library. It does not contain flux-weighted cross sections and, therefore, cannot be input to the ORIGEN-S code. It may be updated by card input or converted to an ORIGEN-S working library. Both input and output libraries can be saved.

4. ORIGEN-S Working Library
   This library is an ORIGEN-S binary library containing one or more sets of burnup-dependent flux-weighted cross sections. It also contains the three-group cross sections for the first set in the library. A multiburnup-dependent library may be produced only by the SAS2 control module (Sect. S2). It can be input to the ORIGEN-S code. It can be made by any one of the following procedures:

   a. direct conversion from a card-image library,
   b. direct conversion from a master library,
   c. an update of a binary library with a weighted AMPX library,
   d. an update of a binary library by card input, or
   e. a fuel assembly depletion analysis by SAS2.

   Either a working or master ORIGEN-S binary library may be input. When a or b is performed, flux-weight factors must be available to the code.

The libraries of 3 and 4 will commonly be called "master library" and "working library," respectively.

5. Weighted AMPX Working Library
This library is an "AMPX working library," used or produced by various AMPX or SCALE system codes. Usually it is the multigroup-weighted-cross-section working library produced by the XSDRNPM-S code (possibly, by execution of SAS2). It will commonly be called "weighted AMPX library" as in 4c above. The data for any nuclide included in the library are assumed to include all important reactions producing a different nuclide. Although the code simply does not change transition data of reactions omitted, the removal cross section for the nuclide is computed as the sum of all of the new (from AMPX library) capture reaction cross sections including the fission cross section.

F6.5.2 PRODUCING LIBRARY DEFAULT TYPES

The "normal" sequence of producing libraries with the COUPLE code is as follows:

1. convert card-image library to a master library;

2. update one master library to another, or a working library, by card input (which may be cross sections or other nuclear data); and

3. update a master library or working library to a working library by using data from a weighted AMPX library.

Options have been added to the COUPLE code so that the binary libraries' input or output to a case may be either a master library or a working library. The type of input library is determined by the code from an ID number. The default type of output library produced in the above cases are, respectively,

1. master library,
2. master library, and
3. working library.

F6.5.3 BINARY LIBRARY ID NUMBER

Each binary library has a "library ID number" obtained by default from the input library or by card input of NEWID (11th entry in 1$ array). Values of NEWID follow the convention:

NEWID < 950 specifies a master library
NEWID > 1000 specifies a working library

A nondefault type of library is obtained by simply specifying the desired type with NEWID.

F6.5.4 LIBRARY SUBDIVISIONS WITHIN A LIBRARY

ORIGEN-S libraries are subdivided (unless deleted by special options) into three different types of libraries: Library 1, 2, and 3, with the following definitions, respectively:

1. Light-Element Library – This library usually contains light elements, cladding, materials of construction in a reactor, and their activation products.

2. Actinide Library – This library usually contains fissile isotopes, other actinides, and their chains of daughter products (those from decay or activation, but not fission products).

3. Fission-Product Library – This library usually contains only fission products, including nuclides directly yielded through fission and their decay and activation products. The term "nuclides" includes isomers of isotopes.

In addition to the division of the library by type of nuclide, given above, the ORIGEN-S card-image library contains separate cross sections for the following (typical) types of reactors:

a. HTGR – High-Temperature Gas-Cooled Reactor
b. LWR – Light-Water Reactor
c. LMFBR – Liquid Metal Fast Breeder Reactor (Pu)
d. MSR – Molten Salt Reactor

F6.5.5 OPTION FOR ADDING NEW PRECURSOR TRANSITIONS

The use of a transition matrix in ORIGEN-S provides the mathematical potential of any nuclide having a transition to any other nuclide. When new card input data or the weighted AMPX library contain a new precursor for a nuclide, it simply requires that the proper matrix element be changed from zero to the new value (cross section or decay constant). However, since the matrix is compressed into an array of only nonzero values, the update is nontrivial. When requested, the code will update the new precursors, requiring a different procedure and slightly more computer time than an update without new precursors. Sometimes the user either is aware that no new precursors are to be added or decides that they are not important for the problem. In such cases, the user may request that the code does not add new precursors. The option is controlled with JADD (4th entry in the 1$ array).

F6.5.6 NUCLIDE OR ISOTOPE IDENTIFICATION NUMBER

A six-digit "nuclide" integer is used to identify each isotope, including its isomeric state. This is called a "nuclide ID No." in the input description. The following equation is used:

$$\text{Nuclide ID No.} = IZ * 10000 + IW * 10 + IS ,$$

where

IZ = the atomic number,
IW = the atomic weight,
IS = 0, for ground state,
IS = 1, for metastable state,
IS > 1, for additional metastable state levels.

F6.5.7 FORMAT OF INPUT DATA

Either the fixed-field, free-field, or user-field type of FIDO input system should be used, except for title cards or supplemental libraries.

Note that each parameter (or entry) is named and defined below in the order that it appears in the data array. If applying fixed-field formats, data entries should be placed in successive data fields. If using free-field form, $$ or ** should be used with the array identifier and at least one space should be skipped between data entries. Each data block contains one or more arrays followed by the data block terminator letter "T," or "iT" where "i" is the data block number.

The normal method of invoking COUPLE at Oak Ridge National Laboratory (ORNL) or the Oak Ridge Gaseous Diffusion Plant (ORGDP) is through the SCALE system. The SCALE driver requires a control card preceding the card input data and an "END" card as the last COUPLE data card (with data for other codes following it, if desired). The complete COUPLE cards are:

```
=COUPLE
(COUPLE code, FIDO-type, data)
END
```

The first and last cards begin in column 1. **Be sure to include** the "END" card. If it is omitted, the output contains only a list of the data.

F6.5.8 COUPLE CODE INPUT PARAMETER DESCRIPTION

No **numerical** data are required if all of the defaults of Data Block 1 are acceptable. In such cases, data sets must be properly assigned in the Job Control Language (JCL) on the mainframe or in the script on a workstation and the following four control data cards (including two for using a SCALE module) are needed to invoke the code and job:

1. =COUPLE, to inform SCALE driver to use code,
2. a blank card to terminate title cards,
3. DONE, for normal job termination message, and
4. END, a data card requirement for SCALE system.

Characters in 1, 3, and 4 are left-adjusted on cards. Also, title cards may be added, as described below.

** All available default values are given in parentheses. **

Data Block 1 – Titles, unit numbers, and case controls. Always required are at least a blank and "DONE" card.

TITLE – Multiple title cards, FORMAT (20A4).

This set of cards provides information added to beginning of Output Library Prologue, which is printed when library is used by ORIGEN-S code. The value of NUMA, in 1$ array, permits retention of prologue cards from the input library. The first blank card terminates the set, which may not exceed 40-NUMA cards. A card with the word "DONE" in first four columns terminates the job. It should follow all cases to be executed. The following includes FIDO-type data array and parameter descriptions with any **default values given in parentheses** after definitions.

-1$ Array - Storage Size Limit (1 entry). This size is the maximum array storage size requested, in computer words. Computer uses smaller of this size and amount available (125,000).

0$ Array - Unit Numbers, required when changing from defaults (9 entries):

1. NOUT - printed output unit numbers (6).
2. NDS - ORIGEN-S card-image library unit number (or first unit number for six separate data sets) (28).
3. JD - "AMPX" type (or XSDRNPM output) weighted library unit number. JD contains the new multigroup (≥3-group) cross sections to be coupled with the input ORIGEN-S library to make new ORIGEN-S library (3).
4. ND - input ORIGEN-S binary library (master or working library) unit number (29).
5. LD - output (updated) ORIGEN-S master library unit number, always used if LBUP=1 (0).
6. MD - output ORIGEN-S working library unit number, used if requested (32).
7. NX - scratch unit number, used if LBUP=1 (17).
8. MX - scratch unit number, sometimes used if LBUP=1 (18).
9. KX - scratch unit number, always used when updating any library (19).

1$ Array - Control Constants (19 entries). This array always required unless all defaults apply. (Request only a single action from either LBIN, LWRK, LBUP, or JEDT per case. Then, new cases may be stacked.)

1. LBIN - 1/0 - input ORIGEN-S library in card-image/binary mode. See note preceding Data Block 3, if LBIN=1 (0).
2. LWRK - 1/0 - do not/do use weighted AMPX library (0).
3. LBUP - 1/0 updated/no (card) update of master library (also, set to 1 for update of working library when NEWID > 1000) (0).
4. JADD - 1/0 - add/do not add new precursor transitions. See Sect. F6.5.5 (0).
5. JEDT - 1/0 - edit only/normal case, no extra edits requested (0).
6. NXX - not used.
7. NMO - current month (as integer) (0).
8. NDAY - current day (0).
9. NYR - current year, in two digits (0). (The ORNL IBM computer will provide date to code, if not entered here.)
10. IDENT - ID number of weighted AMPX library (0).
11. NEWID - Library ID number, required if LBIN = 1 or when not wanting to produce the default-type library. See LWRK, LBUP, and Sect. F6.5.2 for "default" details.

    <950, output master library.

    >1000, output working library.

    0, code increments properly the library ID number and makes default type.

    Also, a master library may simply be converted to a working library if no update action requested (LBIN = 0, LWRK = 1, LBUP = 0) and flux-weighting factors entered in 2* array. Since the default library is always made, even if not saved, always input values for LD and ND when nondefault output requested.

12. IDREF – Nuclide ID number of isotope in weighted AMPX library containing weighting spectrum (proportional to flux) to be used for obtaining flux weights: THERM, RES, and FAST. If 0, and working library is input, code uses old IDREF to refer to new flux spectrum. If 0, and master library is input, code uses flux from first isotope in weighted AMPX library.

13. IEDIN – For requesting edit if JEDT = 1.
    0, no edit
    –1, edits transition cross sections of input working library on ND (0).

14. IEDOU – For requesting edit if JEDIT = 1.
    0, no edit
    –1, edits transition cross sections of output working library on MD (0).

15. NFISW – Number of "substitute" fissile nuclides in output working library entered in 7S Array. Can be applied when JADD = 1 and LWRK = 0, using weighted AMPX library (0).

16. NUMA – Number of title cards obtained from the start of input library prologue to be added to TITLE for output library prologue.

17. NGA1 – Number of energy groups in AMPX data contained in ORIGEN-S thermal group (< 0.5 eV) (1).

18. NGA2 – Number of AMPX resonance groups (1).

19. NGA3 – Number of AMPX fast groups (> 1.0 MeV) (1).

2* Array – Control Parameters (4 entries)

1. TEMP – Reactor moderator average temperature (°C), applied to non-AMPX nuclides. TEMP is not applied when the "1/v absorber material" is included in the weighted AMPX library. For details, see derivation of Eq. (F6.2.8) and feature 3 in Sect. F6.4.2 (303.2).

2. THERM – Thermal flux-weight factor [entries 2, 3, and 4 required only when converting card-image library or a master library (without an update) to a working library]. THERM may be computed as the ratio of the neutron reaction rate for a 1/v absorber reacting with a population of neutrons having a Maxwell-Boltzmann distribution of energies at absolute temperature, T, to the reaction rate with 2200-m/s neutrons:

$$\text{or, THERM} = \sqrt{\frac{\pi}{4}\frac{T_0}{T}}\ , \ T_0 = 293.16\ \text{K}$$

3. RES – Resonance flux per unit lethargy/thermal flux.

4. FAST – Ratio of flux > 1 MeV to fraction of fission spectrum > 1 MeV/ thermal flux. (See Sect. F6.2.1 or F7.6.12 for additional details.)

T – Data Block 1 terminator.

Data Block 2 – Fission Yield Substitutions (if NFISW ≠ 0, 15th entry in 1$ array). This can be used with weighted AMPX library update (LWRK = 0).

7$ Array – Nuclide ID numbers indicating fission yields of one nuclide substituted for another (2*NFISW entries).

Only five fissile nuclides have fission-product yield distributions in the card-image library (see Sect. F7.6.3 in ORIGEN-S Input Description) for these reasons: lack of data, lack of storage, and the relatively small error in fission-product results caused by this limitation. Since cases arise where this is unsatisfactory, the user may, as an approximation, substitute the yield distribution data of one isotope for that of the isotopes which has none given. This is requested by entering pairs of fissile nuclide ID numbers into this array: the first for the nuclide needing yields, and the second for the one to be substituted. The first nuclide must be contained in the weighted AMPX library. Enter NFISW pairs of ID numbers. (Also, see Data Block 8.)

T – Data Block 2 terminator.

IMPORTANT NOTE, WHEN USING OPTION TO UPDATE WITH WEIGHTED AMPX WORKING LIBRARY:

If LWRX = 0 (2nd entry in 1$ Array), a multigroup cross-section update is requested, and the weighted AMPX library is coupled with input ORIGEN-S binary library. **No more data,** described beyond this point, **are required** or permitted for the case. Other cases may be added, or followed with the "DONE" and "END" cards. The remainder of the input description pertains only to converting a card-image to binary library (LBIN = 1) and changing library data by using card input (LBUP = 1). Omit Data Blocks 3, 4, and 5, if LBUP = 1.

Data Block 3 – Converting Card-Image Library. Required if LBIN = 1 (1st entry in 1$ Array): (Identical to Data Block 2 of ORIGEN-S code, except part of it is not used. Note, skip entries not given below.)

3$ Array – Library constants, always required, if data block required (33 entries).

1. NDSET – library data set number. Always set NDSET = NDS (2nd entry in 0$ Array) or –20. Default is NDS.
   –20, six separate data set unit numbers, per 10$ Array.

9. LPU – actinide library data input option (0):
   0, entire actinide data are in NDSET
   N, if cross sections from cards replace library data for "N" nuclides. Nuclide ID numbers read in 6$ Array and new data cards follow Data Block 4.

18. ITMAX ≥ total number of NDSET nuclides, exclusive of LPU (1620)

19. ILMAX ≥ number of light-element nuclides
    –1, omits light-element library (see Sect. F6.5.4 or F7.6.3) (690).

20. IAMAX ≥ number of actinide nuclides
    -1, omits actinide library (105)

21. IFMAX ≥ number of fission-product nuclides
    -1, omits fission-product library (825)

22. IXMAX ≥ total number of reactions from one nuclide to another (6800)

29. NENAC - number of photon actinide library energy groups
    -1, omits library (18)

30. NENLE - number of photon light-element groups
    -1, omits library (12)

31. NENFP - number of photon fission-product groups

    -1, omits library (12)

E - 3$ Array terminator (or enter "0" for entries 32 and 33)

5$ Array - Reactor Library Number, always required

NLIBE - Integer for reactor-type library requested (2):
1/2/3/4 for HTGR/LWR/LMFBR/MSBR Reactors

10$ Data Array - six library unit numbers, if NDSET = -20 (6 entries)

Often this data array is not required since the total library will be contained in six sequential files which all have the same unit number.

1. Light-element nuclear data unit number
2. Actinide nuclear data unit number
3. Fission-product nuclear data unit number
4. Light-element photon data unit number
5. Actinide photon data unit number
6. Fission-product photon data unit number

T - Data Block 3 terminator.

Data Block 4 - Omit, if LPU = 0 in 3$ Array, of if **not** converting a card-image library

6$ Array (LPU entries)

NEWCX - Nuclide ID numbers of the actinide library data read from cards

T - Data Block 4 terminator.

Actinide Card Input:

If LPU > 0 , the LPU cards here override actinide cross sections: format is given in ref. 1 on p. 26.

Data Block 5 – Photon Energy Group Structures and Flag. (Omit if not converting a card-image library.)

35$ Array – Always required (1 entry)

LFLAG – 0, if no more data read in this block and code use default values. These are correct for present ORNL card-image libraries.

1, if more data read in this block. (See ref. 1, Sects. 3.4 and 3.5 for explanation of data used here.)

Warning: Never read photon data here unless a corresponding library has been made (0).

36* Array – Optional (NENAC+1 entries)

EACTGP – Photon energy group structure for actinide nuclides (MeV, in ascending order). Used in printed table column.

37* Array – Optional (NENLE+1 entries)

EGROUP – Photon energy group structure for light-element nuclides (MeV, in ascending order). Used in printed table column.

38* Array – Optional (NENAC entries)

SFGAMA – Photons per fission for ^{235}U in the group structure given by EACTGP.

39* Array – Optional (NENFP+1 entries)

EFPGRP – Photon energy group structure for fission-product nuclides (MeV, in ascending order). Used in printed table column.

Note that any new group structure given in this data block (for printing new group structures) must be exactly the same as the group structure used in making the photon library.

T – Data Block 5 terminator.

Data Block 6 – Number of updated by type and library, required if LBUP = 1 (3rd entry, 1$ Array). This normally produces a master library, which is the default. If wanting to produce a working library, see Sects. F6.5.2 and F6.5.3 and NEWID (11th entry, 1$ Array).

12$ Array – Number of nuclides in the library for which the "nuclear data" [which includes all the data (i.e., Q-values, spontaneous fission, etc.), except cross sections and decay transition constants] are to be updated, completely or in part (3 entries).

LBB – Number of updated nuclides, by library (0)

1. Number in light-element library
2. Number in actinide library
3. Number in fission-product library

Since cross sections and decay constants can be updated elsewhere, this array allows the change of all other nuclide data except the prompt spectra applied during spontaneous fission and separate Y-values, which are updated only from those in the weighted AMPX working library. The updated "nuclear data" are entered in arrays 46$ through 50*, as needed.

13$ Array – Number of fissile nuclides for which substituted fission-product yield distributions are added to library. New yield data for nuclides already having yields are entered in Arrays 71$ through 73*. (1 entry)

NFISM – Number of nuclides for which the substitution mode of using "approximate" yield data is requested (0).

Also requires data in 71$, 72$, and 73* Arrays.

15$ Array – Number of nuclides in the library for which neutron reaction cross sections are to be updated (3 entries).

LBU – Number of updated nuclides, by library (0).

1. Number in light-element library
2. Number in actinide library
3. Number in fission-product library, plus number of fission cross sections, plus number of fissile nuclide to fission-product nuclide reaction transitions, plus NFISM (13$ Array).

The cross-section data are entered in the 71$, 72$, and 73* Arrays, with all fission reactions, entered at the end.

16$ Array – Number of nuclides in the library for which decay transition constants (radioactive half-lives) are to be updated (3 entries).

LBR – Number of updated nuclides, by library (0).

1. Number in light-element library
2. Number in actinide library
3. Number in fission-product library

The radioactive decay constants, $\ln(2)/T_h$ (where T_h is half-life in seconds), and nuclides are entered in 81$, 82$, and 83* Arrays. (Also, see note on DIS in 47* Array.)

T – Data Block 6 terminator.

Data Block 7 – New "Nuclear Data" (nontransitions), required if LBB nonzero in 12$ Array. The entire Data Block 7, including the "T" must be repeated for each nuclide; or, number of times that that Data Block 7 is included in data equals LBB(1) + LBB(2) + LBB(3).

46$ Array – Nuclide definition (2 entries)

1. NUP – nuclide ID number
2. LIB – library containing nuclide
   1, for light-element library

2, for actinide library
3, for fission-product library

Order of the data blocks for updating more than one nuclide requires successive values of LIB to never decrease (i.e., all for LIB = 1 in a group, etc.). No special order is required of nuclide ID numbers within the library group.

47* Array – Nontransition Nuclear Data of Nuclide (8 entries)

1. DIS – Total decay constant. (Note: Updating a transition constant to a daughter nuclide in Data Block 9 causes the code to change DIS, the total decay constant of the parent nuclide, by the same amount. In such instances, do not change DIS here. It is necessary to update DIS only during certain types of data corrections, such as the case when the daughter is missing from the library.)

2. Q – Total energy released by decay as recoverable heat, in MeV.

3. FG – Fraction of energy Q that is from γ-rays (or X rays).

4. AMPC – Radioactivity concentration inhalation guide, RCG_a.

5. WMPC – Radioactivity concentration ingestion guide, RCG_w.

(Entry 6 applies to light elements only.)

6. ABUND – Percent abundance of a naturally occurring isotope.

7. Not used presently.

8. Not used presently.

For each of these 8 entries, the default is the "old" library value. Thus, skip (with "Ai" to the *ith* entry) to entries wanted. If a "0.0" is entered, it changes value to 0.0.

48* Array – Light-Element Photon Yields, may be input if LIB = 1

This array contains the photon yields for nuclide NUP when update is desired and LIB = 1 (in 46$ Array). The units for these spectra are photons per group per disintegration. The group structure may be noted in the ORIGEN-S print of photon release rates. The default is the "old" value. (12 entries, with present card-image libraries; 18 entries with present binary libraries)

49* Array – Actinide Library Photon Yields, if LIB = 2. See note at 48* Array. (18 entries, with present libraries)

50* Array – Fission-Product Photon Yields, if LIB = 3. See note at 48* Array. (12 entries, with present card-image libraries; 18 entries with present binary libraries)

T – Data Block 7 terminator. (repeated, see LBB)

Data Block 8 – New Neutron Reaction Cross-Section Data. This data block is required only if a nonzero value is entered in the 15$ Array. This allows card input of cross sections not coupled from a weighted AMPX library.

71$ Array – Parent Nuclides (LBU(1) + LBU(2) + LBU(3) entries).

ISN1 – Nuclide ID number of the nuclide for which the neutron reaction cross section is to be given. Order these IDs by groups within the library for Library 1, Library 2, and then Library 3. The IDs within a library group may be in any order. (See Sect. F6.5.4 for "Library" meaning.)

Special rules for removal and fission cross sections are given following the "73* Array" description.

72$ Array – Daughter Nuclides. (LBU(1) + LBU(2) + LBU(3) entries)

ISN2 – Nuclide ID number of reaction product of the nuclide at corresponding entry in ISN1. The nuclides ISN1 and ISN2 are required to be in the library specified. The particular reaction or transition does not need to be contained already in the library. If the transition is not in the input library, set JADD = 1 (4th entry, 1$ Array) to have code add all new transition elements. Otherwise, code ignores new transitions and updates remainder of data. Also, see Sect. F6.5.5.

73* Array – Reaction 3-Group Cross Sections. (3*[(LBU(1) + LBU(2) + LBU(3)] entries)

SIGMA – Sets of 3-group cross sections for the reactions ISN1 to ISN2 which are in a corresponding order in 71$ and 72$ Arrays. The three entries for each set should follow the standard ORIGEN-S group definitions:

1. The 2200-m/s neutron reaction cross sections, barns.

2. Resonance integral (>0.5 eV) reaction cross section.

3. Fission-spectrum-averaged cross section of reactions in which the threshold energy of the neutron is above 1.0 MeV.

The third group value must be zero, when the threshold energy is not above 1.0 MeV. Also, the first two group values must be zero, when reactions having thresholds >1.0 MeV apply.

Special 73* Array Rules:

Special meanings can apply to input entered in this data block. Certain rules pertain to removal cross sections and fission reactions, as explained below.

A. Removal Cross Sections

In addition to updating cross sections specified by the transition of ISN1 to ISN2, the user is required to specify the nonfission removal cross section or the sum of all updated and unchanged values of transitions from ISN1. A removal process is indicated by setting ISN2 = ISN1, and the new removal cross section is entered in SIGMA. Even though the value added for removal may always equal the sum of all transition values for that nuclide, this procedure allows for a separate removal cross-section update.

B. Fission Reactions

All fission transitions or cross sections should be included in the last entries of those for Library 3 and counted in the LBU(3) size. The data may have three different meanings, as described below. The data are required to have the following order:

1. Fission-product yields times the fission cross section for a nuclide may be updated. ISN1 is the fissile nuclide and ISN2 is a fission-product nuclide. The cross section in SIGMA should equal the product of the probability of producing ISN2 per fission of ISN1 times the input library (old) fission cross section of ISN1. The yields of various fission products may be given by repeating the fissile nuclide in ISN1. Do not input the updated (for new library) fission-product cross sections times updated yield, even when fission cross sections are being updated (below).

2. Fission cross sections may be updated. No change is made in the fission-product yield distribution, and no yields are added for fissile nuclides previously having no yield data. Enter the fissile nuclide ID number in ISN2 and set ISN1 = -ISN2. Enter the fission cross section in SIGMA. Nuclides for which there are no fission yield data in the library always should be given first in this fission cross-section group.

3. The last NFISM (13$ Array) entries to ISN1 and ISN2 allow the user a special substitution mode for applying fission-product yield data to a fissile nuclide previously having none and, also, updating its fission cross section. Enter the negative of the fissile nuclide ID number (for the nuclide wanted) in ISN1. Enter in ISN2 the nuclide ID number of one of the fissile nuclides for which there are fission-product yields in the input library. (A list of the isotopes having yield data in the card-image libraries is given in Sect. F7.6.3 in the ORIGEN-S Input Description. Also, these fissile nuclides may be determined from a cross-section edit.) Enter the fission cross section in SIGMA. Old values of SIGMA are obtained from entering three zeroes. The fission-product yield distribution for ISN2 will be used for ISN1. While these obviously are not the correct yields, it may improve results obtained with prior libraries in which the yields from the isotope were essentially zero. When a yield above in 1 is being updated in the same case, the old value of the yield is the value used in the substitution. Note the addition of a new fissile nuclide increases the A-matrix array size by the number of fission products produced. An alternative method of yield substitution in which the fission cross section is input from a weighted AMPX library is given in the description of Data Block 2.

T – Data Block 8 terminator.

Data Block 9 – New Radioactive Decay Constant Data. This data block is required only if a nonzero value is entered in the 16$ Array. This allows card input of decay constants and branching ratios of the nuclides.

81$ Array – Parent Nuclides (LBR(1) + LBR(2) + LBR(3) entries).

ISD1 – Nuclide ID number of the nuclide for which the updated decay constant is given. Order these IDs by groups within the library for Library 1, Library 2, and then Library 3. The IDs within a library group may be in any order. (See Sect. F6.5.4 for "Library" meaning.)

82$ Array – Daughter Nuclides (LBR(1) + LBR(2) + LBR(3) entries).

ISD2 – Nuclide ID number of transition product of the nuclide at corresponding entry in ISD1. The nuclides ISD1 and ISD2 are required to be specified in the library. The particular transition, ISD1 to ISD2, does not need to be contained already in the library. If it is not in the input library, set JADD = 1 (4th entry, 1$ Array) to add new transitions. Otherwise, new transitions are ignored. Also, see Sect. F6.5.5. Never set ISD1 = ISD2 since the total decay constant of ISD1 is correct to reflect the change in the decay transition input here. (This process is different for removal cross-section data input in the 71$ and 72$ Arrays.) Also see Data Block 7 to correct total decay constants without changing the transition constants to daughters.

83* Array – Decay Constants (LBR(1) + LBR(2) + LBR(3) entries).

DS – Decay transition constants (or branching fractions times the total decay constant, where there is more than one mode of decay for the nuclide), in s^{-1}. (In terms of T_h, the half-life in seconds, decay constant = $\ln(2)/T_h$.)

T – Data Block 9 terminator.

End of Case Data

New cases may be stacked, starting with Data Block 1. Note, use DONE in TITLE to terminate data for code. Also see Sect. F6.5.6 for invoking COUPLE code and using "END" card.

F6.6 SAMPLE CASES

Three sample cases are presented. These cases are intended to familiarize the user with applying COUPLE. One example (Case 2) shows the method of using COUPLE in the complete procedure of applying associated codes. The input and final answers computed are not intended to be applicable to actual analyses, but the case serves as a guide in the procedure of using the code.

Case 1 – Converting to a Binary Library

Convert the large ORIGEN-S card-image library (Sects. F6.4.1, F6.5.1, and F6.5.8) for the LWR to an ORIGEN-S binary working library on unit number 34. As a second case in the input, stack a request to edit the transition cross sections. Apply JCL with input library on unit number 28. Let THERM, RES, and FAST equal 0.632, 0.333, and 2.0, respectively. Set the library ID number to 1010. The default sizes in the 3$ Array are adequate for the 1609 nuclides in the library being converted. Following are the input data:

```
=COUPLE
- LIBRARY MADE IN TEST CASE 1 -
(blank card)
0$$ A2 28 A6 34 E
1$$ 1 1 A11 1010 E
2** A2 0.632 0.333 2 1T
3T
35$$ 0 5T
(blank card)
0$$ A4 34 E
1$$ A5 1 A13 -1 E 1T
DONE
END
```

(Job execution requires: 43 s on IBM 3090.)

Part of the printed output for this sample is presented on pages F6.6.7 through F6.6.13, inclusive. These are taken from the edit requested in the second case of this sample run. Most of the output from the conversion case is input edits or "debug snapshots" of the start and end of arrays that are stored in the library. Even though this output could be useful, normally it can be ignored. The user may completely delete the debug type of output by compiling subroutines WI and WJ as "dummy" routines. The important output to note in the conversion case is the "Case Completed" statement on the "record-size page" and that no machine error statements are given.

The output examples from the cross-section edit include the library identification page on F6.6.7, the record-size table on F6.6.8, and a single page from the various cross-section edit tables as shown on other pages. Note that the produced nuclide is given under "product" and all target nuclides are listed under "from." The working library effective cross sections for the associated reactions are edited under "total," whereas the three group values of the master library (to be used with problem-dependent flux-weight factors) are listed following the "total." The fission-product edit contains fission cross sections times yield fractions when a fissile nuclide is listed under "from." The Removal Cross-Section table contains all three libraries of nuclides. These values include fission cross sections plus all other capture reaction constants.

Case 2 – Updating With Weighted AMPX Library

Update an ORIGEN-S binary library with the computed cross sections in the weighted AMPX library, produced from a reactor pin cell analysis by the NITAWL-II and XSDRNPM codes, and apply the updated library from COUPLE to an ORIGEN-S irradiation case. Use the composition, geometry, and other parameters needed for the cell calculation as given in the input listed on the following pages. Apply region weighting and collapse the 27 groups to 3 groups as shown.

Apply the library made in Sample Case 1, on unit number 21, as input to COUPLE. Do not add new precursor transitions in data contained in the weighted AMPX library. Specify ^{239}Pu as nuclide applied for obtaining flux weights (although others could be used with equal results). Save one title card in the input ORIGEN-S library, and add title cards shown on the following pages. Set the moderator temperature to 303.2°C. Also, add a case in the COUPLE input to request a cross-section edit of the produced library. Finally, apply the ORIGEN-S case shown using the updated library on unit number 32. The input to all four codes is as follows:

```
=NITAWL
0$$ 82 E 1$$ 0 12 A8 5 E
T
2$$ 1001 5010 5011 40302 92235 92238 95241 94239 94240 94241 94242 8016
3**
  92235  1000. 2 .41212  .2732  3651.9  4.366-4 1 16.  208.4 1 3Z 1.
  92238  1000. 2 .41212  .2732  67.7924 2.352-2 1 16.  3.868 1 3Z 1.
  94239  1000. 2 .41212  .2732  14364.7 1.110-4 1 16.  819.7 1 3Z 1.
  94240  1000. 2 .41212  .2732  60055.6 2.655-5 1 16. 3426.9 1 3Z 1.
  94241  1000. 2 .41212  .2732  131884. 1.209-5 1 16. 7525.5 1 3Z 1.
4**  F550
T
END
=XSDRNPM
   PWR TEST CASE
1$$  2  5  25  1   3  5  18   8  3  1  10 10 0 0 0 E
2$$ -1 3Z E  3$$  1  E
4$$ 1 3 0 -1 E T
13$$ 8R1 1R2 1R3 4R4 4R5
14$$ 8016 92235 92238 94239 94240 94241 94242 95241
  8016 40302 1001 5010 5011 8016
             1001 5010 5011 8016
15**  4.549-2 4.366-4 2.352-2 1.110-4 2.655-5 1.209-5 1.705-6 2.598-7
 1-20   4.252-2  4.836-2 4.28-6 1.78-5 2.418-2
 4.405-2 3.998-6 1.77-5 2.202-2
T
33**   F1.0       T
35**  9I0.0  1I.41212  1I.41738   6I.47572  3I.71187  .74429
36$$  10R1  2R2  2R3  7R4  4R5
39$$  1 2 3 4 5
40$$  5R3
51$$ 5R1 15R2 7R3  T
END
=COUPLE
          *** PWR TEST CASE LIBRARY ***
     *
      (PROBLEM DEPENDENT NEUTRON SPECTRUM FACTORS)
     USED 27 GROUP SCALE LIBRARY AND CONVERTED.........
```

```
0$$ A4 21 A6 32 E
1$$ A12 942390 A16 1 1 1 1 E  2** 303.3 E  T
 EDIT

0$$ A4 32 E  1$$ A2 1 A5 1  A13 -1 E  T
DONE
END
=ORIGENS
1$$  1  T
  SAMPLE CASE 2
3$$  32 A3 1 A16 2 E  T
35$$  0  T
56$$  10  A6 1  A13  2 4 3 0 2 1 1 0   57**   0 0 1-14  E  T
  SAMPLE CASE 2
 MT OF HEAVY METAL CHARGED TO REACTOR
58** F37.5 60$$ 8I88 880 66$$ A5 1 E
73$$ 922350 922380  74** 32000 968000  75$$ F2 T
56$$ F0 T
END
```

(Job execution requires: 62 s on IBM 3090.)

Although sample case 2 produces printed output from four different codes, only output from COUPLE is presented here. Three pages of printed information for the COUPLE case update the ORIGEN-S library. This information is shown on pages F6.6.14, F6.6.15, and F6.6.16. Note that updated effective cross sections for all reaction types in the weighted AMPX library are printed when they are applied in the new library. Also, any reaction that is not used is stated, and the reason for not using it is given. Examples of the requested edit output are not shown, since edit examples appear in the first sample case.

Case 3 – General Nuclear Data Updating

This case is an example of updating a variety of data by card input, only. It includes the three classes of data in the library: the nuclear (nontransition) data, decay transition constants, and cross-section constants. The actual values used may be completely incorrect, but serve as a guide in the input method only.

First input new nuclear data as follows:

1. natural atom % $^{12}C = 98.88$,
2. natural atom % $^{13}C = 1.12$,
3. Q-value of $^{235}U = 4.44$,
4. spontaneous fission $\times A_o$ for $^{240}Pu = 6.36 \times 10^4$,
5. total decay constant of $^{90}Kr = 0.02$,
6. the photon yield in group 4 of $^{90}Kr = 0.105$.

Next, input the following cross-section data, with constants for thermal, resonance, and fast groups, respectively:

1. reaction of ^{242m}Am to ^{243}Am = 350, 130, 0;

2. removal for ^{245}Cm = 2090, 1280, 0;

3. reaction of ^{96}Zr to ^{97}Zr = 540, 0.08, 0;

4. reaction of ^{235}U to ^{95}Zr = 5×10^{-4}, 10^{-4}, 0;

5. fission for ^{245}Cm = 174, 1150, 0;

6. fission-product yields of ^{239}Pu substituted as yields for ^{242m}Am with no change in ^{242m}Am fission cross sections.

Finally, input the following decay transition data:

1. decay constant of ^{14}C to ^{14}N = 3.9×10^{-12},

2. decay constant of ^{242m}Am to ^{242}Am = 6×10^{-10},

3. decay constant of ^{242m}Am to ^{238}Np = 6×10^{-8}.

Input the library made in Sample Case 1 on unit No. 21, set LD = 15, and output a working library on unit No. 32. Permit the code to add new transitions (JADD = 1), and do not save any input library title cards. Edit the new library in a following edit case.

The input is as follows:

```
=COUPLE
 UPDATE EXAMPLE IN COUPLE CODE SAMPLE CASE 3:
 ?? DON'T USE THIS LIBRARY - VALUES ARE INCORRECT??
(INTENDED AS EXAMPLE TO LEARN INPUT METHOD -- ONLY)

 0
0$$ A4 21 15 32 E
1$$ A2 3R1 A11 1020 E 1T
12$$ 2 2 1 13$$ 1 15$$ 0 2 4 16$$ 1 2 0 6T
46$$  60120 1 47** A6 98.88 E T
46$$  60130 1 47** A6  1.12 E T
46$$ 922350 2 47** A2  4.44 E T
46$$ 942400 2 47** A7  6.36+4 E T
46$$ 360900 3 47** 2-2 E 50** A4 0.105 E T
71$$ 952421 962450 400960 922350 -962450 -952421
72$$ 952430 962450 400970 400950  962450  942390
73** 350 130 0 2.09+3 1.28+3 0
 5.4+2 8-2 0 5-4 1-4 0
1.74+2 1.15+3 4Z T
81$$ 60140 952421 952421
82$$ 70140 952420 932380
83** 3.9-12 6-10 6-8 T
EDIT CASE (THIS CARD NOT APPLIED IN LIBRARY)
0$$ A4 32 E 1$$ A2 1 A5 1 A13 -1 E 1T
DONE
END
```

(Job execution requires: 4 s on IBM 3090.)

All pages printed in the update case (except for the FIDO input edits) are shown on pages F6.6.16 through F6.6.20. The nuclear data update page shows both the old and new values. The other data are shown first for the old library and then for the updated library (with headings giving the title cards). The tables have column headings to explain their meanings.

```
        - LIBRARY MADE IN TEST CASE 1 -
ID OF LIBRARY =       1010
* BROAD 3-GROUP FLUX WEIGHTING FACTORS *

        THERM =   0.6320
        RES   =   0.3330
        FAST  =   2.0000
```

	RECORD SIZE
2	20
3	5
4	15
5	1609
6	1609
7	1609
8	6570
9	6570
10	1609
11	101
12	788
13	6570
14	1609
15	101
16	788
17	6570
18	1609
19	101
20	788
21	6570
22	1609
23	6570
24	1609
25	101
26	788
27	1609
28	1609
29	1609
30	1609
31	687
32	101
33	101
34	12
35	18
36	12
37	18
38	8244
39	9852
40	1818

LIGHT ELEMENT LIBRARY OF NEUTRON REACTION CROSS SECTIONS - DATA SET UNIT 34

PRODUCT	FROM	TOTAL	THERMAL	RES.	FAST	FROM	TOTAL	THERMAL	RES.	FAST	FROM	TOTAL	THERMAL	RES.	FAST
H 1	H 2	7.78E-03	0.0	0.0	3.89E-03	HE 3	3.37E+03	5.33E+03	0.0	8.01E-01	LI 6	8.27E-03	0.0	0.0	4.14E-03
	B 10	1.21E-01	1.92E-01	0.0	0.0	N 14	1.48E+00	1.81E+00	8.70E-01	2.14E-02	N 15	3.90E-06	0.0	0.0	1.95E-06
	O 16	3.61E-05	0.0	0.0	1.81E-05	F 19	3.14E-03	0.0	0.0	1.57E-03	NA 23	1.40E-03	0.0	0.0	7.00E-04
	MG 24	2.62E-03	0.0	0.0	1.31E-03	MG 25	3.99E-03	0.0	0.0	1.99E-03	AL 27	6.20E-03	0.0	0.0	3.10E-03
	SI 28	8.00E-03	0.0	0.0	4.00E-03	SI 29	5.41E-03	0.0	0.0	2.70E-03	SI 30	7.90E-06	0.0	0.0	3.95E-06
	P 31	6.20E-02	0.0	0.0	3.10E-02	S 32	1.20E-01	0.0	0.0	6.00E-02	S 33	1.30E+02	2.00E-03	0.0	6.50E+01
	S 34	1.26E-03	0.0	0.0	6.29E-04	CL 35	4.65E-01	4.91E-01	3.68E-01	1.60E-02	CL 37	4.81E-04	0.0	0.0	2.40E-04
	AR 36	1.43E-01	0.0	0.0	7.13E-02	K 39	1.44E-01	0.0	0.0	7.19E-02	K 40	2.78E+00	4.40E+00	0.0	0.0
	CA 40	9.40E-02	0.0	0.0	4.70E-02	CA 42	4.20E-02	0.0	0.0	2.10E-02	CA 43	6.80E-03	0.0	0.0	3.40E-03
	CA 44	1.60E-04	0.0	0.0	7.99E-05	SC 45	1.66E-04	0.0	0.0	8.28E-05	TI 46	2.57E-02	0.0	0.0	1.28E-02
	TI 47	4.40E-02	0.0	0.0	2.20E-02	TI 48	4.20E-04	0.0	0.0	2.10E-04	TI 49	4.60E-03	0.0	0.0	2.30E-03
	TI 50	1.00E-04	0.0	0.0	5.00E-05	V 51	2.01E-04	0.0	0.0	1.00E-04	CR 50	5.07E-02	0.0	0.0	2.54E-02
	CR 52	1.60E-03	0.0	0.0	8.00E-04	CR 53	1.98E-04	0.0	0.0	9.92E-05	CR 54	8.00E-06	0.0	0.0	4.00E-06
	MN 55	8.00E-04	0.0	0.0	4.00E-04	FE 54	1.32E-01	0.0	0.0	6.61E-02	FE 56	1.74E-03	0.0	0.0	8.71E-04
	FE 57	8.03E-04	0.0	0.0	4.02E-04	FE 58	2.00E-05	0.0	0.0	1.00E-05	NI 58	2.24E-01	0.0	0.0	1.12E-01
	NI 60	4.00E-03	0.0	0.0	2.00E-03	NI 61	3.40E-03	0.0	0.0	1.70E-03	NI 62	2.00E-04	0.0	0.0	1.00E-04
	CU 63	1.80E-02	0.0	0.0	9.00E-03	CU 65	7.22E-04	0.0	0.0	3.61E-04	ZR 90	1.80E-03	0.0	0.0	9.00E-04
	ZR 91	5.59E-04	0.0	0.0	2.79E-04	ZR 92	3.20E-04	0.0	0.0	1.60E-04	ZR 94	2.00E-05	0.0	0.0	1.00E-05
	ZR 96	7.99E-07	0.0	0.0	4.00E-07	NB 93	3.60E-03	0.0	0.0	1.80E-03	MO 92	1.24E-02	0.0	0.0	6.20E-03
	MO 94	1.66E-03	0.0	0.0	8.30E-04	MO 95	2.60E-04	0.0	0.0	1.30E-04	MO 96	3.80E-04	0.0	0.0	1.90E-04
	MO 97	2.60E-04	0.0	0.0	1.30E-04	MO 98	1.60E-05	0.0	0.0	7.99E-06	MO100	2.00E-06	0.0	0.0	9.98E-07
	SN114	6.00E-04	0.0	0.0	3.00E-04	SN115	5.99E-04	0.0	0.0	3.00E-04	SN116	1.00E-04	0.0	0.0	5.00E-05
	SN117	1.80E-04	0.0	0.0	9.00E-05	SN118	2.00E-05	0.0	0.0	1.00E-05	SN119	4.00E-05	0.0	0.0	2.00
	PR141	1.90E+00	3.00E+00	0.0	0.0	TB159	1.26E+01	2.00E+01	0.0	0.0	HO165	1.10E+01	1.74E+01	0.0	0.0
	TM169	1.20E+01	1.90E+01	0.0	0.0	BI209	1.14E-05	0.0	0.0	5.70E-06					
H 2	H 1	2.65E-01	3.32E-01	1.66E-01	0.0										
H 3	H 2	3.35E-04	5.30E-04	0.0	0.0	H 4	1.98E+11	0.0	0.0	9.90E+10	HE 3	3.37E+03	5.33E+03	0.0	8.01E-01
	LI 6	6.87E+02	9.40E+02	2.75E+02	5.13E-01										
H 4	H 3	3.79E-06	6.00E-06	0.0	0.0	LI 7	5.16E-02	0.0	0.0	2.58E-02					
HE 4	HE 3	7.96E+02	0.0	2.39E+03	0.0	LI 6	6.87E+02	9.40E+02	2.75E+02	5.13E-01	LI 7	5.16E-02	0.0	0.0	2.58E-02
	BE 9	2.50E-01	0.0	0.0	1.25E-01	B 10	3.00E+03	3.84E+03	1.72E+03	6.37E-01	B 11	1.70E-04	0.0	0.0	8.50E-05
	C 12	9.00E-04	0.0	0.0	4.50E-04	C 13	5.20E-03	0.0	0.0	2.60E-03	N 14	8.32E-02	0.0	0.0	4.16E-02
	N 15	2.61E-05	0.0	0.0	1.30E-05	O 16	1.20E-02	0.0	0.0	6.00E-03	O 17	1.83E-01	2.35E-01	1.05E-01	0.0
	O 18	3.00E-03	0.0	0.0	1.50E-03	F 19	3.43E-02	0.0	0.0	1.71E-02	NE 20	4.00E-02	0.0	0.0	2.00E-02
	NE 21	9.48E-01	1.50E+00	0.0	0.0	NA 23	1.10E-03	0.0	0.0	5.50E-04	MG 24	3.00E-03	0.0	0.0	1.50E-03
	MG 25	3.40E-02	0.0	0.0	1.70E-02	MG 26	6.00E-03	0.0	0.0	3.00E-03	AL 27	1.30E-03	0.0	0.0	6.49E-04
	SI 28	1.48E-03	0.0	0.0	7.39E-04	SI 29	1.28E-02	0.0	0.0	6.40E-03	SI 30	2.00E-04	0.0	0.0	1.00E-04
	P 31	2.58E-03	0.0	0.0	1.29E-03	S 32	3.05E-02	4.00E-03	0.0	1.40E-02	S 33	1.32E+02	1.40E-01	0.0	6.60E+01
	S 34	5.00E-03	0.0	0.0	2.50E-03	CL 35	1.22E-02	7.83E-05	0.0	6.10E-03	CL 37	2.40E-03	0.0	0.0	1.20E-03
	AR 36	8.09E-02	5.51E-03	0.0	3.87E-02	K 39	3.69E-02	4.32E-03	0.0	1.71E-02	K 40	2.46E-01	3.90E-01	0.0	0.0
	CA 40	1.50E-02	2.50E-03	0.0	6.71E-03	CA 42	4.80E-02	0.0	0.0	2.40E-02	CA 43	1.68E-02	0.0	0.0	8.40E-03
	CA 44	6.99E-05	0.0	0.0	3.50E-05	SC 45	7.44E-05	0.0	0.0	3.72E-05	TI 46	1.32E-03	0.0	0.0	6.62E-04
	TI 47	1.10E-02	0.0	0.0	5.50E-03	TI 48	2.21E-05	0.0	0.0	1.10E-05	TI 49	1.62E-03	0.0	0.0	8.09E-04
	TI 50	8.06E-07	0.0	0.0	4.03E-07	V 51	7.07E-06	0.0	0.0	3.54E-06	CR 50	1.30E-03	0.0	0.0	6.50E-04
	CR 52	1.47E-04	0.0	0.0	7.33E-05	CR 53	6.00E-03	0.0	0.0	3.00E-03	CR 54	9.20E-05	0.0	0.0	4.60E-05
	MN 55	2.60E-04	0.0	0.0	1.30E-04	FE 54	4.79E-03	0.0	0.0	2.40E-03	FE 56	6.98E-04	0.0	0.0	3.49E-04
	FE 57	7.00E-03	0.0	0.0	3.50E-03	FE 58	2.00E-05	0.0	0.0	1.00E-05	NI 58	8.84E-04	6.90E-04	0.0	2.24E-04
	NI 59	7.59E+00	1.20E+01	0.0	0.0	NI 60	1.60E-03	0.0	0.0	8.01E-04	NI 61	3.72E-02	4.71E-02	0.0	3.70E-03
	NI 62	1.30E-04	0.0	0.0	6.50E-05	CU 63	1.44E-03	0.0	0.0	7.19E-04	CU 65	3.00E-04	0.0	0.0	1.50E-04
	ZN 64	9.37E-06	1.48E-05	0.0	0.0	ZN 66	1.29E-05	2.04E-05	0.0	0.0	ZN 67	3.79E-06	6.00E-06	0.0	0.0

ACTINIDE LIBRARY OF NEUTRON REACTION CROSS SECTIONS - DATA SET UNIT 34

PRODUCT	FROM	TOTAL	THERMAL	RES.	FAST	FROM	TOTAL	THERMAL	RES.	FAST	FROM	TOTAL	THERMAL	RES.	FAST
RA225	RA224	7.58E+00	1.20E+01	0.0	0.0										
TH229	TH228	7.58E+01	1.20E+02	0.0	0.0										
TH230	TH232	4.40E-04	0.0	0.0	2.20E-04										
TH231	TH230	3.48E+02	2.30E+01	1.00E+03	0.0	TH232	3.20E-02	0.0	0.0	1.60E-02					
TH233	TH232	3.23E+01	7.40E+00	8.30E+01	0.0										
TH234	TH233	1.08E+03	1.50E+03	3.86E+02	0.0										
PA231	PA233	4.40E-04	0.0	0.0	2.20E-04										
PA232	PA231	2.86E+02	2.00E+02	4.80E+02	0.0	PA233	4.32E-02	0.0	0.0	2.16E-02					
PA234M	PA233	1.71E+02	2.20E+01	4.71E+02	0.0										
PA234	PA233	1.63E+02	2.10E+01	4.49E+02	0.0										
U232	U233	6.60E-03	0.0	0.0	3.30E-03	U234	8.80E-05	0.0	0.0	4.40E-05					
U233	U232	1.43E+02	7.80E+01	2.80E+02	0.0	U234	1.44E-02	0.0	0.0	7.20E-03	U235	9.40E-05	0.0	0.0	4.70E-05
U234	U233	7.99E+01	4.90E+01	1.47E+02	0.0	U235	3.00E-02	0.0	0.0	1.50E-02	U236	1.44E-04	0.0	0.0	7.20E-05
U235	U234	2.81E+02	9.50E+01	6.65E+02	0.0	U236	1.30E-02	0.0	0.0	6.50E-03					
U236	U235	1.05E+02	9.80E+01	1.30E+02	0.0	U238	3.00E-04	0.0	0.0	1.50E-04					
U237	U236	7.37E+01	6.00E+00	2.10E+02	0.0	U238	3.00E-02	0.0	0.0	1.50E-02					
U239	U238	8.35E+00	2.73E+00	1.99E+01	0.0										
NP236	NP237	2.60E-03	0.0	0.0	1.30E-03										
NP238	NP237	3.59E+02	1.70E+02	7.56E+02	0.0										
NP240	NP239	1.76E+02	6.00E+01	4.15E+02	0.0										
PU236	PU238	6.00E-05	0.0	0.0	3.00E-05										
PU238	PU239	1.00E-02	0.0	0.0	5.00E-03	PU240	7.00E-05	0.0	0.0	3.50E-05					
PU239	PU238	3.66E+02	5.00E+02	1.50E+02	0.0	PU240	7.00E-03	0.0	0.0	3.50E-03	PU241	1.58E-04	0.0	0.0	7.90E-05
PU240	PU239	4.43E+02	6.32E+02	1.30E+02	0.0	PU241	1.58E-02	0.0	0.0	7.90E-03	PU242	1.48E-04	0.0	0.0	7.40E-05
PU241	PU240	8.97E+02	3.66E+02	2.00E+03	0.0	PU242	1.48E-02	0.0	0.0	7.40E-03					
PU242	PU241	3.94E+02	5.50E+02	1.39E+02	0.0										
PU243	PU242	4.38E+02	1.85E+01	1.28E+03	0.0										
PU245	PU244	1.01E+00	1.60E+00	0.0	0.0										
AM241	AM242M	3.70E-02	0.0	0.0	1.85E-02	AM242	3.70E-02	0.0	0.0	1.85E-02					
AM242M	AM241	2.11E+02	1.50E+02	3.48E+02	0.0										
AM242	AM241	1.09E+03	7.75E+02	1.80E+03	0.0										
AM243	AM242M	1.26E+03	2.00E+03	0.0	0.0										
AM244	AM243	5.66E+02	1.05E+02	1.50E+03	0.0										
CM242	CM243	1.00E-02	0.0	0.0	5.00E-03										
CM243	CM242	1.90E+01	3.00E+01	0.0	0.0										
CM244	CM243	2.93E+02	2.00E+02	5.00E+02	0.0										
CM245	CM244	2.23E+02	1.00E+01	6.50E+02	0.0										
CM246	CM245	2.57E+02	3.43E+02	1.20E+02	0.0										
CM247	CM246	4.11E+01	1.25E+00	1.21E+02	0.0										
CM248	CM247	2.04E+02	6.00E+01	5.00E+02	0.0										

FISSION PRODUCT LIBRARY OF NEUTRON REACTION CROSS SECTIONS - DATA SET UNIT 34

PRODUCT	FROM	TOTAL	THERMAL	RES.	FAST	FROM	TOTAL	THERMAL	RES.	FAST	FROM	TOTAL	THERMAL	RES.	FAST
H 3	U233	7.83E-02	7.09E-02	1.01E-01	0.0	U235	4.49E-02	5.72E-02	2.64E-02	0.0	PU241	1.95E-01	2.59E-01	9.40E-02	0.0
	U238	1.38E-04	0.0	0.0	6.88E-05	PU239	1.86E-01	2.66E-01	5.25E-02	0.0					
CO 72	U233	7.14E-06	6.46E-06	9.18E-06	0.0	U235	1.18E-06	1.50E-06	6.94E-07	0.0	PU241	8.68E-07	1.15E-06	4.18E-07	0.0
	U238	8.91E-09	0.0	0.0	4.46E-09	PU239	8.26E-07	1.18E-06	2.34E-07	0.0					
CO 73	U233	8.59E-08	7.77E-08	1.10E-07	0.0	U235	7.03E-08	8.94E-08	4.13E-08	0.0	PU241	4.49E-09	5.96E-09	2.16E-09	0.0
	U238	5.63E-10	0.0	0.0	2.82E-10	PU239	4.27E-09	6.13E-09	1.21E-09	0.0					
CO 74	U233	2.52E-07	2.28E-07	3.24E-07	0.0	U235	1.74E-07	2.22E-07	1.02E-07	0.0	PU241	1.37E-08	1.82E-08	6.61E-09	0.0
	U238	1.17E-09	0.0	0.0	5.86E-10	PU239	1.30E-08	1.87E-08	3.69E-09	0.0					
CO 75	U233	3.47E-08	3.14E-08	4.46E-08	0.0	U235	2.93E-08	3.73E-08	1.72E-08	0.0	PU241	1.06E-09	1.41E-09	5.12E-10	0.0
	U238	3.62E-10	0.0	0.0	1.81E-10	PU239	1.01E-09	1.45E-09	2.86E-10	0.0					
NI 72	U233	5.92E-04	5.35E-04	7.61E-04	0.0	U235	4.00E-05	5.10E-05	2.35E-05	0.0	PU241	1.27E-04	1.69E-04	6.12E-05	0.0
	U238	1.08E-07	0.0	0.0	5.41E-08	PU239	1.21E-04	1.73E-04	3.42E-05	0.0					
NI 73	U233	6.73E-05	6.09E-05	8.65E-05	0.0	U235	2.01E-05	2.56E-05	1.18E-05	0.0	PU241	7.42E-06	9.86E-06	3.58E-06	0.0
	U238	5.05E-08	0.0	0.0	2.52E-08	PU239	7.06E-06	1.01E-05	2.00E-06	0.0					
NI 74	U233	1.85E-04	1.67E-04	2.38E-04	0.0	U235	5.60E-05	7.12E-05	3.29E-05	0.0	PU241	2.07E-05	2.75E-05	9.99E-06	0.0
	U238	1.21E-07	0.0	0.0	6.04E-08	PU239	1.97E-05	2.83E-05	5.58E-06	0.0					
NI 75	U233	7.77E-05	7.03E-05	1.00E-04	0.0	U235	3.00E-05	3.82E-05	1.76E-05	0.0	PU241	5.08E-06	6.75E-06	2.45E-06	0.0
	U238	1.12E-07	0.0	0.0	5.62E-08	PU239	4.84E-06	6.93E-06	1.37E-06	0.0					
NI 76	U233	1.19E-05	1.08E-05	1.53E-05	0.0	U235	1.01E-05	1.28E-05	5.93E-06	0.0	PU241	7.83E-07	1.04E-06	3.78E-07	0.0
	U238	4.00E-08	0.0	0.0	2.00E-08	PU239	7.46E-07	1.07E-06	2.11E-07	0.0					
NI 77	U233	9.92E-07	8.98E-07	1.28E-06	0.0	U235	1.32E-06	1.68E-06	7.78E-07	0.0	PU241	6.94E-08	9.22E-08	3.35E-08	0.0
	U238	1.61E-08	0.0	0.0	8.07E-09	PU239	6.61E-08	9.47E-08	1.87E-08	0.0					
NI 78	U233	6.90E-08	6.25E-08	8.88E-08	0.0	U235	1.80E-07	2.29E-07	1.06E-07	0.0	PU241	2.28E-09	3.03E-09	1.10E-09	0.0
	U238	2.88E-09	0.0	0.0	1.44E-09	PU239	2.17E-09	3.12E-09	6.15E-10	0.0					
CU 72	U233	1.62E-03	1.46E-03	2.08E-03	0.0	U235	4.98E-05	6.34E-05	2.93E-05	0.0	PU241	5.77E-04	7.67E-04	2.78E-04	0.0
	U238	5.24E-08	0.0	0.0	2.62E-08	PU239	5.49E-04	7.87E-04	1.55E-04	0.0					
CU 73	U233	1.40E-03	1.27E-03	1.81E-03	0.0	U235	1.68E-04	2.13E-04	9.84E-05	0.0	PU241	3.13E-04	4.16E-04	1.51E-04	0
	U238	1.48E-07	0.0	0.0	7.42E-08	PU239	2.98E-04	4.27E-04	8.43E-05	0.0					
CU 74	U233	3.67E-03	3.32E-03	4.72E-03	0.0	U235	5.19E-04	6.60E-04	3.05E-04	0.0	PU241	8.00E-04	1.06E-03	3.86E-04	0
	U238	4.04E-07	0.0	0.0	2.02E-07	PU239	7.61E-04	1.09E-03	2.15E-04	0.0					
CU 75	U233	4.37E-03	3.95E-03	5.62E-03	0.0	U235	8.09E-04	1.03E-03	4.75E-04	0.0	PU241	5.86E-04	7.78E-04	2.82E-04	0.0
	U238	1.01E-06	0.0	0.0	5.05E-07	PU239	5.58E-04	8.00E-04	1.58E-04	0.0					
CU 76	U233	2.08E-03	1.88E-03	2.67E-03	0.0	U235	8.50E-04	1.08E-03	4.99E-04	0.0	PU241	2.77E-04	3.69E-04	1.34E-04	0.0
	U238	9.57E-07	0.0	0.0	4.78E-07	PU239	2.64E-04	3.78E-04	7.47E-05	0.0					
CU 77	U233	5.51E-04	4.98E-04	7.08E-04	0.0	U235	3.49E-04	4.45E-04	2.05E-04	0.0	PU241	8.20E-05	1.09E-04	3.95E-05	0.0
	U238	1.20E-06	0.0	0.0	6.01E-07	PU239	7.81E-05	1.12E-04	2.21E-05	0.0					
CU 78	U233	1.32E-04	1.20E-04	1.70E-04	0.0	U235	1.57E-04	2.00E-04	9.24E-05	0.0	PU241	1.10E-05	1.46E-05	5.30E-06	0.0
	U238	7.36E-07	0.0	0.0	3.68E-07	PU239	1.05E-05	1.50E-05	2.96E-06	0.0					
CU 79	U233	1.38E-05	1.24E-05	1.77E-05	0.0	U235	1.88E-05	2.39E-05	1.10E-05	0.0	PU241	7.00E-07	9.29E-07	3.37E-07	0.0
	U238	1.81E-07	0.0	0.0	9.06E-08	PU239	6.66E-07	9.55E-07	1.88E-07	0.0					
CU 80	U233	9.17E-07	8.29E-07	1.18E-06	0.0	U235	2.70E-06	3.44E-06	1.59E-06	0.0	PU241	4.38E-08	5.82E-08	2.11E-08	0.0
	U238	5.32E-08	0.0	0.0	2.66E-08	PU239	4.17E-08	5.97E-08	1.18E-08	0.0					
CU 81	U233	3.02E-08	2.73E-08	3.88E-08	0.0	U235	1.41E-07	1.79E-07	8.26E-08	0.0	PU241	1.06E-09	1.41E-09	5.11E-10	0.0
	U238	5.81E-09	0.0	0.0	2.90E-09	PU239	1.01E-09	1.45E-09	2.85E-10	0.0					
ZN 72	U233	7.72E-04	6.98E-04	9.92E-04	0.0	U235	1.04E-05	1.32E-05	6.10E-06	0.0	PU241	4.51E-04	5.99E-04	2.17E-04	0.0
	U238	4.03E-09	0.0	0.0	2.02E-09	PU239	4.30E-04	6.16E-04	1.22E-04	0.0					
ZN 73	U233	4.49E-03	4.06E-03	5.77E-03	0.0	U235	2.32E-04	2.95E-04	1.36E-04	0.0	PU241	1.86E-03	2.47E-03	8.97E-04	0.0
	U238	7.59E-08	0.0	0.0	3.80E-08	PU239	1.77E-03	2.54E-03	5.01E-04	0.0					
ZN 74	U233	1.11E-02	1.00E-02	1.42E-02	0.0	U235	8.01E-04	1.02E-03	4.70E-04	0.0	PU241	4.41E-03	5.86E-03	2.13E-03	0.0
	U238	2.33E-07	0.0	0.0	1.16E-07	PU239	4.20E-03	6.02E-03	1.19E-03	0.0					

FISSION CROSS SECTIONS - DATA SET UNIT 34

NUCLIDE	TOTAL	THERMAL	RES.	FAST
TH229	2.02E+01	3.20E+01	0.0	0.0
TH232	3.70E-02	0.0	0.0	1.85E-02
PA231	2.76E+00	0.0	0.0	1.38E+00
U232	1.55E+02	7.70E+01	3.20E+02	0.0
U233	5.80E+02	5.25E+02	7.46E+02	0.0
U234	3.86E+00	0.0	0.0	1.93E+00
U235	4.09E+02	5.20E+02	2.40E+02	0.0
U236	3.24E+00	0.0	0.0	1.62E+00
U237	3.76E+00	0.0	0.0	1.88E+00
U238	5.98E-01	0.0	0.0	2.99E-01
NP236	3.54E+00	0.0	0.0	1.77E+00
NP237	2.45E+00	1.90E-02	0.0	1.22E+00
NP238	1.01E+03	1.60E+03	0.0	0.0
PU236	1.07E+02	1.70E+02	0.0	0.0
PU238	1.94E+01	1.75E+01	2.50E+01	0.0
PU239	1.06E+03	1.52E+03	3.00E+02	0.0
PU240	2.46E+00	0.0	0.0	1.23E+00
PU241	1.11E+03	1.48E+03	5.37E+02	0.0
PU242	2.22E-01	3.50E-02	6.00E-01	0.0
PU243	2.58E+00	0.0	0.0	1.29E+00
AM241	4.18E+00	3.13E+00	0.0	1.10E+00
AM242M	3.80E+03	6.00E+03	0.0	1.83E+00
AM242	1.83E+03	2.90E+03	0.0	0.0
AM243	7.84E-01	4.50E-01	1.50E+00	0.0
AM244	1.45E+03	2.30E+03	0.0	0.0
CM242	3.16E+00	5.00E+00	0.0	0.0
CM243	9.95E+02	6.00E+02	1.85E+03	0.0
CM244	4.92E+00	1.20E+00	1.25E+01	0.0
CM245	1.47E+03	1.73E+03	1.14E+03	0.0
CM247	4.29E+02	1.20E+02	1.06E+03	0.0
CM249	3.16E+01	5.00E+01	0.0	0.0
BK250	1.90E+03	3.00E+03	0.0	0.0
CF249	2.04E+03	1.69E+03	2.92E+03	0.0
CF251	4.17E+03	3.75E+03	5.40E+03	0.0
CF252	5.69E+01	3.20E+01	1.10E+02	0.0
CF253	8.22E+02	1.30E+03	0.0	0.0

REMOVAL CROSS SECTIONS - DATA SET UNIT 34

NUCLIDE	TOTAL	THERMAL	RES.	FAST
H 1	2.65E-01	3.32E-01	1.66E-01	0.0
H 2	8.11E-03	5.30E-04	0.0	3.89E-03
H 3	3.79E-06	6.00E-06	0.0	0.0
H 4	1.98E+11	0.0	0.0	9.90E+10
HE 3	4.16E+03	5.33E+03	2.39E+03	8.01E-01
LI 6	6.87E+02	9.40E+02	2.75E+02	5.17E-01
LI 7	7.73E-02	3.70E-02	7.00E-03	2.58E-02
BE 9	6.87E-01	9.20E-03	4.00E-03	3.40E-01
BE 10	6.32E-04	1.00E-03	0.0	0.0
B 10	3.00E+03	3.84E+03	1.72E+03	6.37E-01
B 11	3.65E-03	5.50E-03	0.0	8.75E-05
C 12	3.55E-03	3.40E-03	1.50E-03	4.50E-04
C 13	6.20E-03	9.00E-04	1.30E-03	2.60E-03
C 14	6.32E-07	1.00E-06	0.0	0.0
N 14	1.62E+00	1.89E+00	9.00E-01	6.30E-02
N 15	4.52E-05	2.40E-05	0.0	1.50E-05
O 16	1.22E-02	1.78E-04	2.70E-04	6.02E-03
O 17	1.83E-01	2.35E-01	1.05E-01	0.0
O 18	3.37E-03	1.60E-04	8.10E-04	1.50E-03
F 19	4.93E-02	9.50E-03	1.76E-02	1.87E-02
NE 20	6.34E-02	3.70E-02	0.0	2.00E-02
NE 21	1.39E+00	2.19E+00	0.0	0.0
NE 22	3.03E-02	4.80E-02	0.0	0.0
NA 22	2.25E+05	4.00E+04	6.00E+05	0.0
NA 23	6.94E-01	9.30E-01	3.11E-01	1.25E-03
MG 24	4.85E-02	5.20E-02	3.00E-02	2.81E-03
MG 25	1.89E-01	1.80E-01	1.11E-01	1.90E-02
MG 26	3.85E-02	3.82E-02	2.50E-02	3.00E-03
MG 27	2.53E-02	4.00E-02	0.0	0.0
AL 27	2.09E-01	2.30E-01	1.70E-01	3.75E-03
SI 28	1.43E-01	1.70E-01	7.80E-02	4.74E-03
SI 29	1.95E-01	2.80E-01	0.0	9.10E-03
SI 30	1.03E-01	1.07E-01	1.06E-01	1.04E-04
SI 31	3.03E-01	4.80E-01	0.0	0.0
P 31	2.05E-01	1.80E-01	8.00E-02	3.23E-02
S 32	4.85E-01	5.34E-01	0.0	7.40E-02
S 33	2.62E+02	1.42E-01	0.0	1.31E+02
S 34	1.58E-01	2.40E-01	0.0	3.13E-03
S 36	9.48E-02	1.50E-01	0.0	0.0
CL 35	3.33E+01	4.35E+01	1.74E+01	2.21E-02
CL 36	6.32E+00	1.00E+01	0.0	0.0
CL 37	2.77E-01	4.33E-01	0.0	1.44E-03
AR 36	4.22E+00	5.01E+00	2.50E+00	1.10E-01
AR 38	6.39E-01	8.00E-01	4.00E-01	0.0
AR 39	3.79E+02	6.00E+02	0.0	0.0
AR 40	5.54E-01	6.60E-01	4.10E-01	0.0

```
 * BROAD 3-GROUP FLUX WEIGHTING FACTORS *
        THERM =  0.6320
        RES   =  0.4085
        FAST  =  3.3460
USER REQUESTED (SEE JADD) THAT ONLY THE NUCLIDE TRANSITIONS PRESENTLY INCLUDED IN
ORIGEN LIBRARY BE UPDATED.
```

CROSS SECTIONS, AVAILABLE FROM AMPX (NORMALIZED TO THERMAL FLUX), BARNS

10010	TO	10020	2.35057E-01
10010	TOT-CAP		2.35057E-01
50100	TO	40100	2.08576E-02
50100	TO	10010	2.08576E-02
50100	TO	40090	3.22542E-03
50100	TO	10020	3.22542E-03
50100	TO	30070	2.70292E+03
50100	TO	20040	2.70308E+03
50100	TO	10030	7.84979E-02
50100	TOT-CAP		2.70302E+03
50110	TO	50100	9.29895E-06
50110	TO	50120	3.57838E-03
50110	TO	40110	1.18664E-06
50110	TO	10010	1.18664E-06
50110	TO	40090	1.05896E-05
50110	TO	10030	1.05896E-05
50110	TO	30080	1.38241E-04
50110	TO	20040	1.38241E-04
50110	TOT-CAP		3.73770E-03
80160	TO	80170	1.25614E-04
80160	TO	70160	8.85364E-05
80160	TO	10010	8.85364E-05
80160	TO	70150	1.66978E-05
80160	TO	10020	1.66978E-05
80160	TO	60130	2.47272E-02
80160	TO	20040	2.47272E-02
80160	TO	80161	3.88287E-03
80160	TOT-CAP		2.49581E-02
922350	TO	922340	2.87877E-02
922350	FISSION		3.97589E+02
922350	NU-SIGF		9.62670E+02
922350	TO	922330	2.76289E-05
922350	TO	922360	9.14510E+01
922350	TO	922351	7.81388E-02
922350	TOT-CAP		4.89069E+02
922380	TO	922370	6.43517E-02
922380	FISSION		9.19647E-01
922380	NU-SIGF		2.59211E+00
922380	TO	922360	4.15928E-04
922380	TO	922390	8.49222E+00
922380	TOT-CAP		9.47663E+00
942390	TO	942380	1.24685E-02
942390	FISSION		9.08939E+02
942390	NU-SIGF		2.61322E+03
942390	TO	942370	2.12484E-05
942390	TO	942360	2.10639E-08
942390	TO	942400	5.03865E+02
942390	TOT-CAP		1.41282E+03

```
942400 TO 942390  5.87321E-03
942400 FISSION    5.54095E+00
942400 NU-SIGF    1.73759E+01
942400 TO 942380  5.73133E-05
942400 TO 942410  1.36930E+03
942400 TOT-CAP    1.37484E+03
942410 TO 942400  7.36547E-02
942410 FISSION    9.81816E+02
942410 NU-SIGF    2.88062E+03
942410 TO 942390  1.22634E-04
942410 TO 942420  3.22479E+02
942410 TOT-CAP    1.30437E+03
942420 TO 942410  2.39414E-02
942420 FISSION    4.25043E+00
942420 NU-SIGF    1.33318E+01
942420 TO 942400  2.91069E-04
942420 TO 942430  3.26620E+02
942420 TOT-CAP    3.30895E+02
952410 FISSION    1.23801E+01
952410 NU-SIGF    3.99540E+01
952410 TO 952420  1.05712E+03
952410 TOT-CAP    1.06950E+03

THE REACTION   80160 TO  80161 WAS NOT USED, BECAUSE   80161 IS NOT IN LIBRARY., (IN SUBR POOL)

THE REACTION  922350 TO 922351 WAS NOT USED, BECAUSE  922351 IS NOT IN LIBRARY., (IN SUBR POOL)

THE REACTION  942390 TO 942370 WAS NOT USED, BECAUSE  942370 IS NOT IN LIBRARY., (IN SUBR POOL)

THE FISSION PRODUCT TRANSITIONS FOR  942400 WERE NOT USED.  LIBRARY FISSILE NUCLIDES ARE
  922330   922350   942410   922380   942390

USE SUBSTITUTE NUCLIDE IN BLOCK 8 DATA.  OR, UPDATE WITH NEW FISSION YIELD DATA.

THE FISSION PRODUCT TRANSITIONS FOR  942420 WERE NOT USED.  LIBRARY FISSILE NUCLIDES ARE
  922330   922350   942410   922380   942390

USE SUBSTITUTE NUCLIDE IN BLOCK 8 DATA.  OR, UPDATE WITH NEW FISSION YIELD DATA.

THE FISSION PRODUCT TRANSITIONS FOR  952410 WERE NOT USED.  LIBRARY FISSILE NUCLIDES ARE
  922330   922350   942410   922380   942390

USE SUBSTITUTE NUCLIDE IN BLOCK 8 DATA.  OR, UPDATE WITH NEW FISSION YIELD DATA.

                    CASE COMPLETED.  DATE,  11/18/1981
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NUCLEAR (NON-TRANSITION) DATA UPDATED

     DIS*
            KR 90          2.1446E-02 TO        2.0000E-02

       Q
            U235           4.4180E+00 TO        4.4400E+00

      FG

     AMPC

     WMPC

     ABUND
            C 12           9.8890E+01 TO        9.8880E+01
            C 13           1.1100E+00 TO        1.1200E+00

     SPONF
            PU240          1.0119E+05 TO        6.3600E+04

   ALPHAN

         ANY PHOTON LIBRARY UPDATES FOLLOW
           LIGHT ELEMENTS
           FISSION PRODUCTS
             KR 90         0.0         TO       1.0500E-01 FOR GROUP  4
           ACTINIDES

* UPDATES THE DECAY CONSTANT, BUT NO DECAY TRANSITIONS.  APPLIES TO CASES IN WHICH
  TRANSITION IS NOT UPDATED (SUCH AS, WHEN PRODUCT NUCLIDE IS NOT IN LIBRARY).

    NUCLEAR DATA UPDATE DONE
```

* * INPUT LIBRARY DATA BEING MODIFIED * *

- LIBRARY MADE IN TEST CASE 1 -

NUCLIDE	DECAY CONSTANT	BRANCH TO	TRANSITION CONSTANT
C 14	3.8332E-12	N 14	3.8332E-12
AM242M	1.4450E-10	AM242	1.4378E-10
AM242M	1.4450E-10	NP238	7.2251E-13

* * OUTPUT LIBRARY DATA UPDATED * *

UPDATE EXAMPLE IN COUPLE CODE SAMPLE CASE 3:
?? DON'T USE THIS LIBRARY - VALUES ARE INCORRECT??
(INTENDED AS EXAMPLE TO LEARN INPUT METHOD — ONLY)

NUCLIDE	DECAY CONSTANT	BRANCH TO	TRANSITION CONSTANT
C 14	3.9000E-12	N 14	3.9000E-12
AM242M	6.0600E-08	AM242	6.0000E-10
AM242M	6.0600E-08	NP238	6.0000E-08

* * INPUT LIBRARY DATA BEING MODIFIED * *

- LIBRARY MADE IN TEST CASE 1 -

..THERMAL GROUP CROSS SECTIONS..

NUCLIDE	REMOVAL	FISSION	BRANCH TO	TRANSITION CONSTANT
AM242M	8.0000E+03	6.0000E+03	AM243	2.0000E+03
CM245	2.0700E+03			
ZR 96	5.3000E-02	0.0	ZR 97	5.3000E-02
U235	6.1800E+02	5.2000E+02	ZR 95	1.5444E-01
CM245	2.0700E+03	1.7270E+03		

..RESONANCE GROUP CROSS SECTIONS..

NUCLIDE	REMOVAL	FISSION	BRANCH TO	TRANSITION CONSTANT
AM242M	0.0	0.0	AM243	0.0
CM245	1.2600E+03			
ZR 96	7.0000E-02	0.0	ZR 97	7.0000E-02
U235	3.7000E+02	2.4000E+02	ZR 95	7.1280E-02
CM245	1.2600E+03	1.1400E+03		

..FAST GROUP CROSS SECTIONS..

NUCLIDE	REMOVAL	FISSION	BRANCH TO	TRANSITION CONSTANT
AM242M	1.8477E+00	1.8281E+00	AM243	0.0
CM245	0.0			
ZR 96	0.0	0.0	ZR 97	0.0
U235	1.4893E-02	0.0	ZR 95	0.0
CM245	0.0	0.0		

```
          * * OUTPUT LIBRARY DATA UPDATED * *

 UPDATE EXAMPLE IN COUPLE CODE SAMPLE CASE 3:
 ?? DON'T USE THIS LIBRARY - VALUES ARE INCORRECT??
(INTENDED AS EXAMPLE TO LEARN INPUT METHOD -- ONLY)

                    ..THERMAL GROUP CROSS SECTIONS..

 NUCLIDE     REMOVAL      FISSION    BRANCH TO    TRANSITION CONSTANT

  AM242M  8.0000E+03  6.0000E+03      AM243          3.5000E+02
  CM245   2.0900E+03
  ZR 96   5.3000E-02  0.0             ZR 97          5.4000E+02
   U235   6.1800E+02  5.2000E+02      ZR 95          5.0000E-04
  CM245   2.0900E+03  1.7400E+02

                    ..RESONANCE GROUP CROSS SECTIONS..

 NUCLIDE     REMOVAL      FISSION    BRANCH TO    TRANSITION CONSTANT

  AM242M  0.0         0.0             AM243          1.3000E+02
  CM245   1.2800E+03
  ZR 96   7.0000E-02  0.0             ZR 97          8.0000E-02
   U235   3.7000E+02  2.4000E+02      ZR 95          1.0000E-04
  CM245   1.2800E+03  1.1500E+03

                    ..FAST GROUP CROSS SECTIONS..

 NUCLIDE     REMOVAL      FISSION    BRANCH TO    TRANSITION CONSTANT

  AM242M  1.8477E+00  1.8281E+00      AM243          0.0
  CM245   0.0
  ZR 96   0.0         0.0             ZR 97          0.0
   U235   1.4893E-02  0.0             ZR 95          0.0
  CM245   0.0         0.0
   FISSION PRODUCT YIELD DATA OF NUCLIDE PU239  APPLIED AS YIELD DATA FOR NUCLIDE AM242M
```

F6.7 I/O UNIT REQUIREMENTS

Listed below are all of the possible I/O unit number requirements in the JCL for executing the COUPLE code. The user should determine which I/O units to include in the JCL from the options selected in the input to the case (see Sect. F6.5). For example, when selecting the option to update by applying a weighted AMPX library, units N5, N6 (with NOUT = N6), JD, ND, MD, and KX are required. Default values are shown when not zero.

UNIT	DEFAULT	PURPOSE
N5	5	Card input (fixed)
N6	6	FIDO edits (fixed)
NOUT	6	Printed output
LIBDEC	27	Decay data base (fixed)
NDS	28	Card-image ORIGEN-S library input
NDSET	0	Usually, default is NDSET=NDS
JD	3	Weighted AMPX library
ND	29	ORIGEN-S binary library input
LD	0	ORIGEN-S master library output
MD	32	ORIGEN-S working library output
NX	17	Scratch data set
MX	18	Scratch data set
KX	19	Scratch data set

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Computing Applications Division

ORIGEN-S: SCALE SYSTEM MODULE TO CALCULATE FUEL DEPLETION, ACTINIDE TRANSMUTATION, FISSION PRODUCT BUILDUP AND DECAY, AND ASSOCIATED RADIATION SOURCE TERMS

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ABSTRACT

ORIGEN-S computes time-dependent concentrations and source terms of a large number of isotopes, which are simultaneously generated or depleted through neutronic transmutation, fission, radioactive decay, input feed rates, and physical or chemical removal rates. The calculations may pertain to fuel irradiation within nuclear reactors, or the storage, management, transportation, or subsequent chemical processing of removed fuel elements. The matrix exponential expansion model of the ORIGEN code is unaltered in ORIGEN-S. Essentially all features of ORIGEN were retained, expanded, or supplemented within new computations.

The primary objective of ORIGEN-S, as requested by the SCALE sponsors at the U.S. Nuclear Regulatory Commission (NRC), is to make it possible for the calculations to utilize the multi-energy-group cross sections from any currently processed standardized ENDF/B data base. This purpose has been implemented through the prior execution of codes within either the SCALE system or the AMPX system, developed at Oak Ridge National Laboratory (ORNL). These codes compute flux-weighted cross sections, simulating conditions within any given reactor fuel assembly, and convert the data into a library that can be input to ORIGEN-S. Time-dependent libraries may be produced, reflecting fuel composition variations during irradiation. Some of the other objectives included in ORIGEN-S are the convenience of free-form input, the flexible dimensioning of storage to avoid size restrictions on libraries or problems, the computation of gamma and neutron source spectra in any requested energy group structure, the application of a more complete standardized photon data base, the determination of neutron absorption rates for all nuclides, and the integration of fission product energies and sources over any decay interval, by applying the Volterra multiplicative integral method.

Presented in the document are detailed and condensed input instructions, model theory, available features, range of applicability, brief subroutine descriptions, sample input, and I/O requirements. Some of the revisions to this document reflect several major modifications to the code. The computation of neutron source spectra for UO_2 or α-emitters in borosilicate glass has been added. Also, the calculation of neutron source strengths has been significantly improved. Another major change is the addition to the types of data that may be saved for later use. These data can be input and used by PLORIGEN (Sect. F15), a code for plotting ORIGEN-S results. ORIGEN-S was converted to FORTRAN 77 and has been implemented on the IBM 3090 mainframe, the IBM RS/6000 and DEC ULTRIX workstations, the CRAY X-MP, and a 4867 PC at ORNL. The code was modified to automatically determine machine precision in an attempt to have a machine-independent version. Indeed, identical versions (except for translating the FORTRAN source to lower or upper case) exist on the IBM mainframe and workstation and CRAY computers.

ORIGEN-S is a functional module in the SCALE system and is one of the modules invoked in the SAS2 control module, or it may be applied as a "stand-alone" program. It can be used in nuclear reactor and processing plant design studies, burnup credit evaluations, radiation safety analyses, and environmental assessments.

The MS-DOS PC code, ORIGNATE, was developed to substantially simplify ORIGEN-S case input preparation. It uses state-of-the-art PC techniques, such as pull-down menus and context-sensitive help message boxes.

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F7.1 INTRODUCTION

The original version of the ORIGEN program[1] was developed by the Chemical Technology Division of ORNL for use in computing the compositions and radioactivity of fission products, cladding materials, and fuel materials in LWRs, LMFBRs, MSBRs, and HTGRs. The primary advantage of ORIGEN over earlier burnup codes is its capability to treat the full isotopic transition matrix rather than a limited number of transmutation chains. This capability in ORIGEN arises from a clever application of the matrix exponential method.

In ORIGEN the storage normally required for the isotopic transition matrix is greatly reduced by packing the nonzero elements and then using three vectors of indexing information to subsequently locate the particular elements. Also, ORIGEN performs the matrix exponential expansion with a recursion relation which requires the storage of only two vectors in addition to the solution vector.

The version of ORIGEN applied in the SCALE system, ORIGEN-S, has several improvements over the original program. The code has been modified to include dynamic storage allocation, free-form input processing, and flexible dimensioning. However, the most significant improvement has been the development of the COUPLE (see Sect. F6) program which updates the ORIGEN cross-section libraries with constants processed for user-specified systems by the NITAWL-II and XSDRNPM modules (see Sects. F2 and F3, respectively). The original ORIGEN program had four cross-section libraries designed for the analysis of fuel irradiated in each of the four reactor types mentioned above. In several instances, the cross sections and resonance integrals in these libraries were adjusted[1] to obtain agreement between calculated and measured fuel mass balances.

In the SCALE system, basic microscopic cross-section data, originally processed from the ENDF/B files,[2] is further processed through NITAWL-II and XSDRNPM for the particular reactor fuel-pin lattice specified by the user. Then the COUPLE module updates the ORIGEN-S cross-section libraries with the neutron flux-averaged constants from XSDRNPM. Thus, the SCALE system provides the capability of executing ORIGEN with data that have been rigorously processed for a particular fuel assembly with a user-specified irradiation history.

The primary application of ORIGEN in the SCALE system is in the SAS2 shielding analytical sequence (see Sect. S2). This sequence includes an ORIGEN-S analysis of the fuel irradiation and decay history, thereby providing the neutron and photon radiation source terms for shielding analyses. Also, ORIGEN-S can be executed on a stand-alone basis in SCALE with a complete set of user-specified input. Through this procedure, the SCALE system user can select ORIGEN options such as chemical processing features and additional output options.

Traditionally, the decision to select different models (i.e., matrix exponential or Bateman equation solution methods) by ORIGEN-S has been dependent upon the precision of the floating-point computer word of the machine. Specifically, the size of the word precision controls the number of nuclides that are removed from the transition matrix and require the Bateman equation model. This dependence would require either code modifications that were nontrivial in changing the code for other machines with less precision or the use of unnecessary CPU time for machines with greater precision. An attempt has been made to make the computing of the machine word precision and the subsequent calculation of all model selection parameters entirely automated in ORIGEN-S. Also, the literal floating-point sizes used for specific variable definitions have been changed to be within the size limits of most workstations and PCs. More extensive input and output coding have been added so that the code would execute, in general, on most types of computers. In addition, the code has been converted to FORTRAN 77. These changes have been an attempt to make ORIGEN-S machine-independent.

The purpose of this section is to document the SCALE system version of ORIGEN. Particular emphasis is given to the description of the analytical procedures employed in ORIGEN-S and to providing guidance to the user on the applicability of these procedures to various problems.

F7.2 THE ANALYTICAL METHOD

F7.2.1 STATEMENT OF THE PROBLEM

In determining the time dependence of nuclide concentrations, ORIGEN-S is primarily concerned with developing solutions for the following equation:

$$\frac{dN_i}{dt} = \text{Formation Rate} - \text{Destruction Rate} - \text{Decay Rate} . \qquad \text{(F7.2.1)}$$

ORIGEN[1] considers radioactive disintegration and neutron absorption (capture and fission) as the processes appearing on the right-hand side of Eq. (F7.2.1). The time rate of change of the concentration for a particular nuclide, N_i, in terms of these phenomena can be written as

$$\frac{dN_i}{dt} = \sum_j \gamma_{ji}\sigma_{f,j}N_j\phi + \sigma_{c,i-1}N_{i-1}\phi + \lambda_i'N_i' - \sigma_{f,i}N_i\phi - \sigma_{c,i}N_i\phi - \lambda_i N_i , \qquad \text{(F7.2.2)}$$

where (i = 1, ... I), and

$\sum_j \gamma_{ji}\sigma_{f,j}N_i\phi$ is the yield rate of N_i due to the fission of all nuclides N_j;

$\sigma_{c,i-1}N_{i-1}\phi$ is the rate of transmutation into N_i due to radiative neutron capture by nuclide N_{i-1};

$\lambda_i'N_i'$ is the rate of formation of N_i due to the radioactive decay of nuclides N_i';

$\sigma_{f,i}N_i\phi$ is the destruction rate of N_i due to fission;

$\sigma_{c,i}N_i\phi$ is the destruction rate of N_i due to all forms of neutron capture (n,γ, n,α, n,p, n,2n, n,3n);

$\lambda_i N_i$ is the radioactive decay rate of N_i.

Equation (F7.2.2) is written for a homogeneous medium containing a space-energy-averaged neutron flux, ϕ, with flux-weighted average cross sections, σ_f and σ_c, representing the reaction probabilities. In reality, the flux as a function of space, energy, and time is dependent upon the nuclide concentrations. ORIGEN assumes that the space-energy-averaged flux can be considered constant over time steps Δt. Similarly, ORIGEN assumes that a single set of flux-weighted neutron cross sections is adequate for use over the entire fuel exposure time. For a given time step, these assumptions are necessary if Eq. (F7.2.2) is to be treated as a first-order, linear differential equation.

In the SCALE system we retain these assumptions for time steps Δt and thus maintain the applicability of the ORIGEN mathematical treatment. However, for successive time steps, Δt_k, Δt_{k+1}, ..., Δt_n, we provide the capability of determining updated values for the space-energy-averaged flux and, therefore, for the flux-weighted cross sections.[2] These values are the results of NITAWL-II and XSDRNPM lattice cell analyses based on updated values for the nuclide concentrations.

F7.2.2 SOLUTION WITH THE MATRIX EXPONENTIAL METHOD

Proceeding with the description of the ORIGEN-S analytical model, for all nuclides N_i, Eq. (F7.2.2) represents a coupled set of linear, homogeneous, first-order differential equations with constant coefficients. As such, Eq. (F7.2.2) can be written in matrix notation as

$$\underset{\sim}{\dot{N}} = \underset{\approx}{A}\,\underset{\sim}{N}, \tag{F7.2.3}$$

where $\underset{\sim}{N}$ is a vector of nuclide concentrations and $\underset{\approx}{A}$ is the transition matrix containing the rate coefficients for radioactive decay and neutron absorption. Equation (F7.2.3) has the known solution

$$\underset{\sim}{N} = \exp(\underset{\approx}{A}t)\underset{\sim}{N}(o), \tag{F7.2.4}$$

where $\underset{\sim}{N}(o)$ is a vector of initial nuclide concentrations. Analogous to a series expansion for the exponential function, the matrix exponential function, $\exp(\underset{\approx}{A}t)$, appearing in Eq. (F7.2.4), is defined as

$$\exp(\underset{\approx}{A}t) \equiv \underset{\approx}{I} + \underset{\approx}{A}t + \frac{(\underset{\approx}{A}t)^2}{2} + \ldots = \sum_{m=o}^{\infty} \frac{(\underset{\approx}{A}t)^m}{m!}, \tag{F7.2.5}$$

with $\underset{\approx}{I}$ being the unit matrix. Equations (F7.2.4) and (F7.2.5) constitute the matrix exponential method, which yields a complete solution to the problem. However, in certain instances, difficulties occur in generating accurate values of the matrix exponential function. Under these circumstances, alternative procedures using either the generalized Bateman equations[3] or Gauss-Seidel iterative techniques are applied. These alternative procedures will be discussed after the completion of the exposition on the matrix exponential method.

A straightforward solution of Eq. (F7.2.4) through the expansion in Eq. (F7.2.5) would require the in-core storage of the complete transition matrix. To avoid this storage requirement, a recursion relation has been developed. Substituting for the matrix exponential function in Eq. (F7.2.4) we have

$$\underset{\sim}{N} = \left[\underset{\approx}{I} + \underset{\approx}{A}t + \frac{(\underset{\approx}{A}t)^2}{2!} + \frac{(\underset{\approx}{A}t)^3}{3!} + \ldots\right]\underset{\sim}{N}(o). \tag{F7.2.6}$$

The recursion relation may be observed by considering the solution of Eq. (F7.2.6) for a particular nuclide, N_i. The result is a series of terms which arise from the successive post-multiplication of the transition matrix by the vector of nuclide concentration increments produced from the computation of the previous terms. Within the accuracy of the series expansion approximation, physical values of the nuclide concentrations are obtained by summing a converged series of these vector terms. The elements of the transition matrix, a_{ij}, are the first-order rate constants for the formation of nuclides i from nuclides j. The solution in terms of these rate constants is written as

$$N_i = N_i(o) + t\sum_j a_{ij}N_j(o) + \frac{t}{2}\sum_k \left[a_{ik}t\sum_j a_{kj}N_j(o)\right] + \frac{t}{3}\sum_m \left\{a_{im} \times \frac{t}{2}\sum_k \left[a_{mk}t\sum_j a_{kj}N_j(o)\right]\right\} + \ldots, \quad \text{(F7.2.7)}$$

where the range of indices, j, k, m, is 1 to M for a size M × M of matrix $\underset{\sim}{A}$.

The recursion relation is developed from Eq. (F7.2.7) by defining the terms C_i^n as

$$C_i^o \equiv N_i(o),\ C_i^{n+1} = \frac{t}{n+1}\sum_j a_{ij}C_j^n, \quad \text{(F7.2.8)}$$

which yields the solution for N_i as

$$N_i = \sum_{n=o}^{\infty} C_i^n. \quad \text{(F7.2.9)}$$

The use of Eq. (F7.2.9) in obtaining the solution for the system of nuclides given in Eq. (F7.2.4) requires the storage of only two vectors, $\underset{\sim}{C}^n$ and $\underset{\sim}{C}^{n+1}$, in addition to the current value of the solution.

Various tests are conducted in ORIGEN to ensure that the summations indicated in Eq. (F7.2.9) do not lose accuracy owing to relative magnitudes or small differences between positive and negative rate constants. Nuclides with large rate constants are removed from the transition matrix and treated separately. For example, in the decay chain A → B → C, if the decay constant for B is large, a new rate constant is inserted in the matrix for A → C. This technique was originally employed by Ball and Adams.[4]

The determination of which transitions are to be reduced from the matrix involves the calculation of the matrix norm. The norm of the matrix $\underset{\sim}{A}$ is defined by Lapidus and Luus[5] as being the smaller of the maximum-row absolute sum and the maximum-column absolute sum. That is, the norm, [A], is given by

$$[A] = \min\left\{\max\sum_i |a_{ij}|,\ \max\sum_j |a_{ij}|\right\}. \quad \text{(F7.2.10)}$$

In order to maintain precision in performing the summations of Eq. (F7.2.9), the matrix norm is used to balance the user-specified time step, t, with the precision associated with the word length employed in the machine calculation. Lapidus and Luus have shown that the maximum term in the summation for any element in the matrix exponential function cannot exceed $([A]t)^n/n!$ where n is the largest integer not larger than [A]t. In the ORIGEN program, [A]t is restricted by

$$[A]t \le -2\ \ell n(0.001) = 13.8155. \quad \text{(F7.2.11)}$$

This value restricts the size of the maximum term to approximately 10^5. The IBM mainframe (e.g., the IBM 3090) operating system retains 16 significant decimal figures when performing double-precision arithmetic. Given the maximum term of 10^5 and 16 significant-figure precision, ORIGEN can maintain five significant-

figure accuracy in values as small as 10^{-6}. The precision of ORIGEN calculations on non-IBM mainframe computers can be easily determined for any particular value of machine precision.*

The restriction (F7.2.11) is maintained by removing nuclides from the transition matrix when $e^{-dt} < 0.001$, where "-d" is the diagonal element for the nuclide. Since "d" is the sum of decay constant plus the product of total absorption cross section and flux, the sum of the absolute values in the column containing d cannot exceed 2d. It always equals 2d when all of its daughter nuclides are contained in the matrix (i.e., its loss rate equals its product transition rate). Even though the sum of the absolute values in the row containing d may exceed 2d, the norm [A] defined by Eq. (F7.2.10) never exceeds twice the maximum value of d in the reduced matrix. Thus, $[A]t \le 2dt = -2\,\ell n(e^{-dt}) \le -2\,\ell n(0.001)$. Note that nuclides are considered short-lived if their effective half-lives are less than about 10% of the time interval ($1/2^{10} = 1/1024 \doteq 0.001$).

A generalized equation may be derived for computing the maximum norm of $\underset{\approx}{A}t$, given m, the number of significant figures of the computer word for a specified machine, and j, the required number of significant figures in all results. It is preferred to cast the equation in terms of the maximum absolute diagonal element, $|dt|$, where $[A] = 2|d|$ holds true for any $\underset{\approx}{A}$ constructed by ORIGEN-S. The "largest term of the series" is known for any "answer," $\exp(-[A]t)$, of the series summation. Thus, for any values of j and m, the required condition of significance can be stated by the inequality

$$(\text{Largest term in series}) \times 10^{-m} \le (\text{series answer}) \times 10^{-j},$$

which is

$$\max_n \frac{|2dt|^n\, 10^{-m}}{n!} \le \exp(-|2dt|)10^{-j} \qquad \text{(F7.2.12)}$$

or

$$\max_n \frac{|2dt|^n \exp(|2dt|)}{n!} \le 10^{m-j}.$$

This equation may be solved by trial for $|2dt|$ and $\exp(|dt|)$, applying the fact that n is the greatest integer in $|2dt|$. Let m = 7, to represent the single-precision word of the IBM mainframe computer. The results for two values of j are calculated in the following:

For j = 4,

$$[A]t = |2dt| = 4.27; \quad \exp(-|dt|) = 0.12;$$

Also, for j = 2.6,

$$[A]t = |2dt| = 6; \quad \exp(-|dt|) = 0.05.$$

---

*The calculation of machine precision and the correction in 13.8155 for each machine has been automated by ORIGEN-S.

In the current version of ORIGEN-S, all nuclides for which $\exp(-\lambda dt) < 0.001$ are removed from $\underset{\sim}{A}$ and must be handled by alternative procedures. Increasing this restriction value to 0.12, or 0.05, would result in more computer time and possibly other problems.

Another use of the matrix norm in ORIGEN is in the determination of the number of terms required for convergence of the series in Eq. (F7.2.9). A quantity k which is derived from [A]t is used in determining a trial value of this parameter as the largest integer in 7/2 k + 5. For most applications, this algorithm yields a number of terms sufficient to limit the summation error to less than 0.1%. For example, for a value of [A] equal to 13.8155, the summation will be carried to 53 terms. The 53rd term will be less than 6.4×10^{-10}, which is less than 0.1% of 10^{-6}.

In certain applications where the interest is in nuclide concentrations computed over long transmutation chains, the above algorithm may not be adequate for yielding accurate concentrations for those nuclides near the end of the chain that are significantly affected by those near the beginning. For this reason, the algorithm in ORIGEN-S has been modified to set the number of expansion terms to the maximum of 7/2 [A] + 5, 21, or a user-specified value. As guidance in determining a value to specify, the user can consider the ZA number of the nuclides on the extremities of the chain of interest, $Z_1A_1 \rightarrow Z_2A_2$, and use the expression

$$n = |Z_2 - Z_1| + |A_2 - A_1| + 5, \qquad \text{(F7.2.13)}$$

which will generate a 5-term correction to the first estimate of the concentration of Z_2A_2.

F7.2.3 SOLUTION TO THE NUCLIDE CHAIN EQUATIONS

As discussed in Sect. F7.2.2, nuclides with short half-lives are removed from the transition matrix and treated separately. This separate treatment involves the solution of the nuclide chain equations. In conjunction with maintaining the transition matrix norm below the prescribed level, a queue is formed of the short-lived precursors of each long-lived isotope. These queues extend back up the several chains to the last preceding long-lived precursor. The queues include all nuclides whose half-lives (loss due to decay and neutron absorption) are less than 10% of the time interval. A generalized form of the Bateman equations developed by Vondy[6] is used to solve for the concentrations of the short-lived nuclides at the end of the time step.

For an arbitrary forward-branching chain, Vondy's form of the Bateman solution is given by

$$N_i = N_i(o)e^{-d_i t} + \sum_{k=1}^{i-1} N_k(o)\left[\sum_{j=k}^{i-1} \frac{e^{-d_j t} - e^{-d_i t}}{(d_i - d_j)} a_{j+1,j} \prod_{\substack{n=k \\ n\neq j}}^{i-1} \frac{a_{n+1,n}}{d_n - d_j}\right], \qquad \text{(F7.2.14)}$$

where $N_1(o)$ is the initial concentration of the first precursor, $N_2(o)$ that of the second precursor, etc. As in Eq. (F7.2.7), a_{ij} is the first-order rate constant and d_i is equal in magnitude to the diagonal element, or $d_i = -a_{ii}$. Bell[1] has recast Vondy's form of the solution through multiplication and division by $\prod_{n=k}^{i-1} d_n$. Rearranging terms he obtains

$$N_i = N_i(o)e^{-d_i t} + \sum_{k=1}^{i-1} N_k(o) \prod_{n=k}^{i-1} \frac{a_{n+1,n}}{d_n} \left[\sum_{j=k}^{i-1} d_j \frac{e^{-d_j t} - e^{-d_i t}}{(d_i - d_j)} \prod_{\substack{n=k \\ n \neq j}}^{i-1} \frac{d_n}{d_n - d_j} \right]. \quad \text{(F7.2.15)}$$

The first product over isotopes n is the fraction of atoms that remain after the kth particular sequence of decays and captures. If this product falls less than 10^{-6}, the contribution of this sequence to the concentration of nuclide i is neglected. Indeterminate forms arising when $d_i = d_j$ or $d_n = d_j$ are evaluated using L'Hopital's rule. These forms occur when two isotopes in a chain have the same diagonal element.

The solution given by Eq. (F7.2.15) is applied to calculate all contributions to the "queue end-of-interval concentrations" of each short-lived nuclide from initial concentrations of all others in the queue described above. The beginning-of-interval concentrations of long-lived or stable daughter products are augmented by the appropriate contribution from all nuclides of the queue divided by e^{-dt}, where d is its diagonal element. Even though dividing by e^{-dt} produces a more correct concentration of the long-lived nuclide, it overpredicts its daughter concentrations. This adjustment is normally a small fraction of these concentrations in the usual reactor applications intended for the code (i.e., the ratio of the concentrations of long-lived daughters to that of their short-lived precursors is large).

Equation (F7.2.15) is applied in making adjustments to certain elements of the final transition matrix, which now excludes the short-lived nuclides. The value of the element must be determined for the new transition between the long-lived precursor and the long-lived daughter of a short-lived queue. The element is adjusted such that the end-of-interval concentration of the long-lived daughter calculated from the single link between the two long-lived nuclides (using the new element) is the same as what would be determined from the chain including all short-lived nuclides. The method assumes zero concentrations for precursors to the long-lived precursor. The computed values asymptotically approach the correct value with time as successive time intervals are executed. (For this reason, at least five to ten time intervals are recommended in place of one or two during a typical reactor exposure period. Larger intervals during the decay of discharged fuel are reasonable, because long-lived nuclides have built up by that time.)

In the instance that a short-lived nuclide has a long-lived precursor, an additional solution is required. First, the amount of short-lived nuclide i due to the decay of the initial concentration of long-lived precursor j is calculated as

$$N(t)_{j-i} = N_j(o)a_{ij} \frac{e^{-a_{jj}t}}{a_{ii} - a_{jj}} \quad \text{(F7.2.16)}$$

from Eq. (F7.2.15) with $a_{kk} = d_k$ and assuming $\exp(-d_i t) << \exp(-d_j t)$. However, the total amount of nuclide i produced depends upon the contribution from the precursors of precursor j, in addition to that given by Eq. (F7.2.16). The quantity of nuclide j not accounted for in Eq. (F7.2.16) is denoted by $N_j'(t)$, the end-of-internal concentration minus the amount which would have remained had there been no precursors to nuclide j,

$$N_j'(t) = N_j(t) - N_j(o)e^{-a_{jj}t}. \quad \text{(F7.2.17)}$$

Then the short-lived daughter and subsequent short-lived progeny are assumed to be in secular equilibrium with their parents, which implies that the time derivative in Eq. (F7.2.2) is zero.

$$\dot{N}_i = o = \sum_j a_{ij} N_j . \qquad \text{(F7.2.18)}$$

The "queue end-of-interval concentrations" of all the short-lived nuclides following the long-lived precursor are augmented by amounts calculated with Eq. (F7.2.15). The concentration of the long-lived precursor used in Eq. (F7.2.17) is that given by Eq. (F7.2.16). The set of linear algebraic equations given by Eq. (F7.2.18) is solved by the Gauss-Seidel iterative technique. This algorithm involves an inversion of the diagonal terms and an iterated improvement of an estimate for N_i through the expression

$$N_i^{k+1} = - \frac{1}{a_{ii}} \sum_{j \neq i} a_{ij} N_j^k . \qquad \text{(F7.2.19)}$$

Since short-lived isotopes are usually not their own precursors, this iteration often reduces to a direct solution.

F7.2.4 THE NONHOMOGENEOUS CASE

So far, in the discussion of the analytical model applied in ORIGEN-S, we have considered the solution of the homogeneous equation, Eq. (F7.2.3). This equation is applicable to reactor fuel burnup calculations, and therefore its solution is of primary interest for incorporation into the SCALE system analytical sequences. However, an additional capability resides in the ORIGEN program to consider an externally imposed time rate-of-change for the nuclide concentrations. This capability would be applicable to various phases of fuel reprocessing. Mathematically, the consideration of such rate changes results in a nonhomogeneous form of Eq. (F7.2.3),

$$\dot{\underset{\sim}{N}} = \underset{\approx}{A}\, \underset{\sim}{N} + \underset{\sim}{B} . \qquad \text{(F7.2.20)}$$

For a user-specified set of rate changes, $\underset{\sim}{B}$, the particular solution of Eq. (F7.2.20) is sought to be added to the solution of the homogeneous equation, Eq. (F7.2.3). As before, the matrix exponential method is used for the long-lived nuclides and secular equilibrium is assumed for the short-lived nuclides. Adopting an unknown vector quantity $\underset{\sim}{C}$, a trial function for the particular solution is constructed as

$$\underset{\sim}{N} = \sum_{m=o}^{\infty} \left[\frac{(\underset{\approx}{A}t)^m}{(m+1)!} \right] \underset{\sim}{C} t . \qquad \text{(F7.2.21)}$$

Substitution of Eq. (F7.2.21) into Eq. (F7.2.20), expanding and differentiating terms yield

$$\underset{\approx}{I}\underset{\sim}{C} + \underset{\approx}{A}\underset{\sim}{C}t + \frac{\underset{\approx}{A}^2\underset{\sim}{C}}{2!}t^2 + \ldots = \underset{\approx}{A}\underset{\approx}{I}\underset{\sim}{C}t + \frac{\underset{\approx}{A}^2\underset{\sim}{C}}{2!}t^2 + \ldots + \underset{\sim}{B}. \qquad \text{(F7.2.22)}$$

Cancellation of like terms on opposite sides of Eq. (F7.2.22) indicates that the trial function satisfies Eq. (F7.2.20), with the unknown vector $\underset{\sim}{C}$ equal to the forcing function $\underset{\sim}{B}$. Therefore, the complete solution for Eq. (F7.2.20) is written as

$$\underset{\sim}{N} = \sum_{m=o}^{\infty} \frac{(\underset{\approx}{A}t)^m}{m!}\underset{\sim}{N}(o) + \sum_{m=o}^{\infty} \frac{(\underset{\approx}{A}t)^m}{(m+1)!}\underset{\sim}{B}t \qquad \text{(F7.2.23)}$$

For the second term in Eq. (F7.2.23), a new recursion relation is developed in the same manner as Eqs. (F7.2.6) through (F7.2.9). The resulting recursion relation is

$$N_i^P = \sum_{n=1}^{\infty} D_i^n, \qquad \text{(F7.2.24)}$$

where

$$D_i^1 = b_i t; \quad D_i^{n+1} = \frac{t}{n+1}\sum_j a_{ij} D_j^n.$$

For the short-lived nuclides, the secular equilibrium equations are modified to become

$$\dot{N}_i = 0 = \sum_j a_{ij} N_j + b_i. \qquad \text{(F7.2.25)}$$

Again, the Gauss-Seidel iterative method is applied to determine the solution. The complete solution to the system of equations (F7.2.20) is given by the sum of the homogeneous solutions described earlier and the particular solutions described here.

F7.2.5 TIME DEPENDENCE OF THE NEUTRON FLUX

The ORIGEN user has the option of specifying a fixed value for the neutron flux or the specified power. The SCALE analytical sequences call for the power per fuel assembly history and fuel volume data from which the specific power is determined. The average neutron flux over the time interval is obtained from the specific power, microscopic fission cross sections, and an approximate expression for the fissioning nuclide concentrations as a function of time.

Assuming a value of 200 MeV per fission, the specific power due to fission is

$$P = 3.2 \times 10^{-17} \sum_i N_i \sigma_{f,i} \phi , \qquad \text{(F7.2.26)}$$

where P is the specific power in MW/cm^3, 3.2×10^{-17} MW equals 200 MeV/s, $\sum_i N_i \sigma_{f,i}$ is the total macroscopic fission cross section of the fuel in cm^{-1}, and ϕ is the instantaneous value of the neutron flux in neutrons/cm^{2}s. With a specified constant power level, the flux as a function of time varies only with the concentrations of the fissionable nuclides. Inverting Eq. (F7.2.26), the flux as a function of time is written as

$$\phi(t) = 3.125 \times 10^{16} P/\Sigma(t) , \qquad \text{(F7.2.27)}$$

where $\Sigma(t) = \sum_i N_i(t) \sigma_{f,i}$.

Next, $\Sigma(t)$ appearing in Eq. (F7.2.27) is expanded in a Taylor series about $t = 0$,

$$\phi(t) = 3.125 \times 10^{16} P \left[\Sigma(o)^{-1} - \frac{t\dot{\Sigma}(o)}{\Sigma(o)^2} + \frac{t^2}{2} \frac{(2\dot{\Sigma}(o)^2 - \Sigma(o)\,\ddot{\Sigma}(o))}{\Sigma(o)^3} + \ldots \right] \qquad \text{(F7.2.28)}$$

and Eq. (F7.2.26) for $t = 0$ is substituted for the specific power to obtain

$$\phi(t) = \phi(o) \left[1 - t\frac{\dot{\Sigma}(o)}{\Sigma(o)} + \frac{t^2}{2} \frac{(2\dot{\Sigma}(o)^2 - \Sigma(o)\ddot{\Sigma}(o))}{\Sigma(o)^2} + \ldots \right] . \qquad \text{(F7.2.29)}$$

To obtain the average flux over the time interval, t, Eq. (F7.2.29) is integrated over the interval, $0 \le t' \le t$, and divided by t, resulting in

$$\bar{\phi}(o) = \phi(o) \left[1 - \frac{t}{2} \frac{\dot{\Sigma}(o)}{\Sigma(o)} + \frac{t^2}{6} \frac{(2\dot{\Sigma}(o)^2 - \Sigma(o)\ddot{\Sigma}(o))}{\Sigma(o)^2} + \ldots \right] \qquad \text{(F7.2.30)}$$

The time derivatives of the macroscopic fission cross sections evaluated at the beginning of the time interval correspond directly to the time derivatives of the fissionable nuclide concentrations. From Eq. (F7.2.3) it is seen that the time derivative of the nuclide concentrations can be expressed as a vector quantity which is directly related to the nuclide concentrations by the transition matrix. Furthermore, the second derivative can also be expressed in terms of the nuclide concentrations as

$$\ddot{\underset{\sim}{N}}(o) = \underset{\approx}{A}\,\dot{\underset{\sim}{N}}(o) = \underset{\approx}{A}^2 \underset{\sim}{N}(o) \qquad \text{(F7.2.31)}$$

Evaluation of Eq. (F7.2.30) using Eq. (F7.2.31) provides the average flux as being a vector sum of flux components arising from the fissioning of the various nuclides at the beginning of each time interval. In the computer program, the estimation for the average flux includes only the first two terms of Eq. (F7.2.30) for all time intervals except the first. At the first interval, the second derivative term will be significant because the first derivative term will be zero for many nuclides.

When the user specifies a fixed value of the neutron flux, the average power over the time interval is obtained from the following expression:

$$P = 3.2 \times 10^{-17} \phi(o) [\Sigma(o) + \dot{\Sigma}(o)t/2 + \ddot{\Sigma}(o)t/6 + ...] . \quad \text{(F7.2.32)}$$

Equation (F7.2.32) is obtained from Eq. (F7.2.26) through a Taylor series expansion and time integration as discussed above. Since only a few terms are retained in these expansions, they are accurate only for slowly varying functions of time. Therefore, the user may have to reduce the specified time step to ensure an accurate calculation of the average flux or the average power. If either of these quantities differs from the value at the beginning of time step by more than 20%, a warning is printed to use smaller time steps.

The coefficient of the neutron flux in Eq. (F7.2.26) was derived with the assumption of a constant value of 200 MeV/fission for fissioning events with all nuclides. This value was programmed into the original version of ORIGEN and its use remains as a user-specified option in ORIGEN-S. However, the default option in ORIGEN-S is to determine the average energy per fission on the basis of the neutron absorption occurring during each time step. In this method, the coefficient in Eq. (F7.2.26) is replaced with the quantity

$$1.6 \times 10^{-19} \sum_{ij} Q_{ij} N_i \sigma_{ij} .$$

Here, the total thermal energy from neutron absorption is the sum of the yields, Q_{ij}, for nuclides i and reaction types j (fission, radiative capture, etc.) weighted by their probability of occurrence. Note that energy carried off by neutrinos is not included. Values for the thermal yields for 24 fissile isotopes and other important nuclides have been taken from ENDF/B files. A thermal yield of 5 MeV is used for radiative capture of nuclides which are not important or for which ENDF/B data are not available. This is a typical value of known thermal yields, and the total contribution from these nuclides is usually less than 0.3% of the average energy per fission.

During the 3-year burnup cycle in a light-water reactor, the average energy per fission may change by several percent as the higher mass number actinides become more important. However, these changes are very small during the normal-size time step. Therefore, as in the case of the microscopic cross sections, the thermal yields are considered to be constant over each time step and they do not enter into the time derivatives in Eqs. (F7.2.28) through (F7.2.32).

F7.2.6 SPECTRAL DEPENDENCE OF THE NEUTRON CROSS SECTIONS

ORIGEN data libraries include cross sections for three neutron energy ranges: a thermal range below 0.5 eV, a resonance energy range extending up to 1 MeV, and a fast energy range above 1 MeV. When running ORIGEN-S as a stand-alone module, the user specifies the factors THERM, RES, and FAST. THERM is used to adjust the 2200-m/s cross sections in the library for a thermal neutron spectrum corresponding to a known value of the reactor moderator temperature. RES and FAST are used to weight the epithermal cross sections relative to the thermal cross sections in forming one-group values.

Among the input parameters for the SCALE system control modules, the user specifies an average fuel temperature for Doppler broadening fuel cross sections and a moderator temperature for use in selecting the thermal scattering kernel. These functions are performed in the NITAWL-II module in preparing a working cross-section library. Subsequent to the flux calculation in XSDRNPM, the moderator temperature is also used in the COUPLE module to calculate a value of THERM, following the model of Westcott:[7]

$$\text{THERM} = \sqrt{\frac{\pi}{4}\frac{T_o}{T}}, T_o = 293.16\ \text{K}. \qquad \text{(F7.2.33)}$$

Another procedure for deriving THERM may be applied in COUPLE when the user specifies the inclusion of a special 1/v absorber material in the XSDRNPM flux calculation. See Sect. F7.6.12 for details of this method. Values for RES and FAST are calculated as

$$\text{RES} = \sum_{E_g \geq 0.5\,\text{eV}}^{E_g \leq 1\,\text{MeV}} \phi_g \qquad \left[\ell n\left(\frac{10^6}{0.5}\right) \sum_{E_g \leq 0.5\,\text{eV}} \phi_g\right] \qquad \text{(F7.2.34)}$$

and

$$\text{FAST} = 1.45 \sum_{E_g \geq 1\,\text{MeV}} \phi_g \qquad \sum_{E_g \leq 0.5\,\text{eV}} \phi_g . \qquad \text{(F7.2.35)}$$

In Eqs. (F7.2.34) and (F7.2.35), ϕ_g are the groupwise fluxes calculated in XSDRNPM. The logarithmic term in the expression for RES corresponds to the lethargy increment over the resonance energy range. Its inclusion in Eq. (F7.2.34) accommodates the use of the infinitely dilute resonance integral, which is the ORIGEN library convention for this energy range.

The quantity 1.45 in the definition of FAST is equal to the reciprocal of the fraction of the fission neutron spectrum above 1 MeV. It appears here to correct for the initial averaging of the tabulated fast cross sections (thresholds above 1 MeV) over the entire energy range.

Having calculated THERM, RES, and FAST, COUPLE combines the XSDRNPM output and these terms to produce three-group constants that are consistent with the ORIGEN calculation of reaction rates based upon the total thermal flux.[1]

$$\text{SIGTH} = \sum_{E_g \leq 0.5\,\text{eV}} \sigma_g \phi_g \qquad \left[\text{THERM} \sum_{E_g \leq 0.5\,\text{eV}} \phi_g\right] \qquad \text{(F7.2.36)}$$

$$\text{RITH} = \sum_{E_g \geq 0.5\,\text{eV}}^{E_g \leq 1\,\text{MeV}} \sigma_g \phi_g \qquad \left[\text{RES} \sum_{E_g \leq 0.5\,\text{eV}} \phi_g\right] \qquad \text{(F7.2.37)}$$

$$\text{SIGMEV} = \sum_{E_g \geq 1\,\text{MeV}} \sigma_g \phi_g \qquad \left[\text{FAST} \sum_{E_g \leq 0.5\,\text{eV}} \phi_g\right] \qquad \text{(F7.2.38)}$$

This procedure preserves the relative importance of the three energy ranges as calculated by XSDRNPM. Furthermore, the procedure maintains the capability of properly treating the 2200-m/s cross sections, infinitely dilute resonance integrals, and fission spectrum averaged fast cross sections from the ORIGEN libraries. This capability is necessary for those nuclides which are *not* having their cross sections updated with XSDRNPM calculated values.

F7.2.7 THE VOLTERRA MULTIPLICATIVE INTEGRAL SOLUTION

The primary problem solved by ORIGEN-S is the determination of time-dependent nuclide concentrations. Even though the matrix exponential solution applied by Bell[1] was described previously in this section, an alternative matrix operator method formulated by Lee[8] for calculating radioactive decay is presented here. This model produces (1) the "instantaneous concentrations" of nuclides similar to that determined by Eq. (F7.2.4) and (2) the "time-integrated concentrations" from the integration of Eq. (F7.2.4) over any specified time interval. The second model is useful in computing either the total disintegrations or the total energy released from fission products during various cooling intervals. These integrals more correctly simulate counting measurements, total heat, or radiation exposure than those derived from directly "averaging" the instantaneous values from the matrix exponential method. The results from "averaging" can be either precise or erroneous, depending on the prevailing conditions of the problem. To avoid encumbering the matrix operations described in this section, we denote a matrix by a capital letter and a vector by a capital letter that is underscored with a single wave. In stating the problem, again, we assume a linear, homogeneous, first-order differential matrix equation, as in Eq. (F7.2.3)

$$\dot{\underset{\sim}{N}}(t) = A\underset{\sim}{N}(t) . \qquad \text{(F7.2.39)}$$

Substituting C = At into Eq. (F7.2.4), the solution to Eq. (F7.2.39) becomes

$$\underset{\sim}{N}(t) = e^{C}\underset{\sim}{N}(o) = \sum_{k=0}^{\infty} \frac{C^k}{k!}\underset{\sim}{N}(o) . \qquad \text{(F7.2.40)}$$

The integral of Eq. (F7.2.40) over the limits o to t can be written as

$$\int_o^t \underset{\sim}{N}(t)dt = \int_o^t e^{C}\underset{\sim}{N}(o)dt = A^{-1}(e^{C} - I)\underset{\sim}{N}(o) , \qquad \text{(F7.2.41)}$$

with I as the unit matrix. The inverted matrix A^{-1} can be eliminated, however, by recasting Eq. (F7.2.40)

$$\begin{aligned} \underset{\sim}{N}(t) &= \underset{\sim}{N}(o) + e^{C}\underset{\sim}{N}(o) - I\underset{\sim}{N}(o) \\ &= \underset{\sim}{N}(o) + CC^{-1}(e^{C} - I)\underset{\sim}{N}(o) \\ &= \underset{\sim}{N}(o) + CD(C)\underset{\sim}{N}(o) \end{aligned} \qquad \text{(F7.2.42)}$$

and defining

$$D(C) = C^{-1}(e^{C} - I) = \sum_{k=0}^{\infty} \frac{C^k}{(k+1)!} . \qquad \text{(F7.2.43)}$$

Since D(C) exists, Eq. (F7.2.42) becomes an alternate of Eq. (F7.2.40) as a solution to Eq. (F7.2.39). Also, applying $A^{-1} = C^{-1}t$ and Eqs. (F7.2.41) and (F7.2.43), the solution to the integral is

$$\underset{\sim}{G}(t) = \int_0^t \underset{\sim}{N}(t)dt = C^{-1}t(e^{C} - I)\underset{\sim}{N}(o) = D(C)\underset{\sim}{N}(o)t \tag{F7.2.44}$$

It is shown in Sect. F7.2.2 that as a result of computer "round-off," the inclusion of C^k in summations of Eqs. (F7.2.40) and (F7.2.43) for a norm $[C] >> 1$, as defined by Eq. (F7.2.10), will cause computer computations to become completely erroneous. However, applying the laws of exponentiation, we may scale C by repeatedly dividing C by 2 until it satisfies the condition that all its eigenvalues are bounded by unity. Then, e^C can be evaluated using a recursion relationship to scale each intermediate function of $C/2^n$ back up to D(C). If H is defined as the properly scaled matrix of C,

$$H = 2^{-p}C, \tag{F7.2.45}$$

then the integer p may be determined from[8]

$$p > \ell n\left(\sum_{i=1}^{m}\sum_{j=1}^{m} c_{ij}^2\right) \qquad 2\ \ell n(2) \tag{F7.2.46}$$

and also the following condition for the norm, defined by either Eq. (F7.2.10) or the Euclidean norm:

$$[H] \le \frac{1}{2}. \tag{F7.2.47}$$

Applying H in Eq. (F7.2.43) in place of C,

$$D(H) = H^{-1}(e^{H} - I) = \sum_{k=o}^{\infty} \frac{H^k}{(k+1)!} \tag{F7.2.48}$$

It has been shown[8] that

$$D(C) = D(2^pH) = D(2^{p-1}H)[I + \frac{1}{2}(2^{p-1}H)D(2^{p-1}H)] \tag{F7.2.49}$$

is true for all $p \ge 0$, since $D(2^{n+1}H)$ can be determined by

$$\begin{aligned} D(2^{n+1}H) &= (2^{n+1}H)^{-1}(e^{2^{n+1}H} - I) \\ &= (2^nH)^{-1}(e^{2^nH} - I)(2I + e^{2^nH} - I)\cdot\frac{1}{2} \\ &= D(2^nH)[I + \frac{1}{2}(2^nH)(2^nH)^{-1}(e^{2^nH} - I)] \\ &= D(2^nH)[I + \frac{1}{2}(2^nH)D(2^nH)], \end{aligned} \tag{F7.2.50}$$

and Eq. (F7.2.49) is true for p = 0, 1 and has the same form as Eq. (F7.2.50). Thus, D(C) can be evaluated. Lee[8] applies the Euclidean norm, which is the square root of the summation term in Eq. (F7.2.46). Bell maintains precision by applying the "min-max" norm of Eq. (F7.2.10) used in the matrix theory by Lapidus and Luus.[5] In ORIGEN-S the maximum of these two differently defined norms is applied, so that either required size of the norm can be applied in the error analysis. Further, the integer p is increased by "1," changing the final norm to

$$[H] \leq \frac{1}{4}. \qquad \text{(F7.2.51)}$$

The request for the "integral option" in the input to ORIGEN-S invokes the application of the above model, computing both the time-integrated solution by Eq. (F7.2.44) and the regular or instantaneous solution by Eq. (F7.2.42). The method is restricted to the calculation of fission products decay. This restriction is the result of computer core storage limitations. The direct application of the model requires the storage of five matrices. The size of these matrices for the complete set of ORIGEN-S libraries (light elements, actinides, etc.) would be 1700 × 1700, requiring as much as 1.45×10^7 additional double-precision words or 116,000 kB. However, the storage requirement can be drastically reduced for the fission product decay matrix. Since there are no isotopes having alpha decay in the fission product library, each nuclide can decay only to those nuclides which have identical mass numbers.* The complete transition matrix A for any set of nuclides of the same mass number has a small size (i.e., the maximum of 12 × 12). The code simply converts the large, sparse transition matrix for the entire problem to a set of full-valued submatrices corresponding to transitions with common nuclide mass numbers. Each submatrix and its corresponding subvector is processed by the above model during a separate execution loop. Thus, the core storage requirements are minimal. Since neutron reaction products can have a mass number differing from those included in the submatrix of the target nuclides, the method is not applicable to neutron irradiation. The primary purpose of the method is the integration of nuclide activities over specified decay intervals. The computation of the solutions given by Eqs. (F7.2.42) and (F7.2.44) is performed in double-precision arithmetic, which normally provides about 16 decimal digits of precision on the IBM mainframe (e.g., IBM 3090) computers. The proof that a particular computer calculation retains a specified precision requires an evaluation of the effect of the truncation of some of the right-hand bits of the computer word during the subtraction process. A similar evaluation of the matrix exponential method is discussed in Sect. F7.2.2. For the integral method, a precision analysis indicated that the truncation effect is limited to the following two sources of error: (1) the effect of omitting terms in the series of D(H) defined by Eq. (F7.2.48) and (2) the effect of truncation or round-off error in computing D(H), each $D(2^nH)$, G(t), and N(t).

F7.2.7.1 Absolute Error in D(H) from Omitting Series Terms

First consider the errors in computing D(H). Since D(H) is computed from a finite number of terms, M, the elements d_{ij} of D(H) have an absolute error $E^M(d_{ij})$. The algorithm in ORIGEN-S sets M = 10 and applies

*The model is limited to only the fission-product libraries that have not had delayed neutron branching fractions added, as shown in a COUPLE case in Sect. M6. After a day or less from discharge, all delayed neutron production is insignificant for almost all problems of interest.

$$D^{M}(H) = \left[I + \frac{H}{2}\left(I + \frac{H}{3}\left\{I + \ldots\left[I + \frac{H}{M-1}\left(I + \frac{H}{M}\right)\right]\right\}\right)\right] \qquad \text{(F7.2.52)}$$

from the M*th* term backwards. Then the absolute error is

$$E^{M}(d_{ij}) \le \frac{[H]^{M+1}}{(M+2)!} = \frac{1}{4^{M+1}(M+2)!} \le 5 \times 10^{-16}. \qquad \text{(F7.2.53)}$$

This does not include round-off error, which is evaluated later.

F7.2.7.2 Relative Errors in D(H)

Since it is possible that an element $d_{ij} < 5 \times 10^{-16}$, it appears necessary to examine the relative errors, $R^{M}(d_{ij})$. Through matrix element arithmetic, diagonal and off-diagonal relative errors were determined as

$$R^{M}(d_{ii}) \le 6 \times 10^{-16} \qquad \text{(F7.2.54)}$$

$$R^{M}(d_{i,i-1}) \le 5 \times 10^{-14} \qquad \text{(F7.2.55)}$$

and in general, assuming no branching,

$$R^{M}(d_{ij}) \le \frac{\sum_{s=j}^{i-1} h_{ss}}{d_{ij}} \sum_{r=j}^{i} \frac{h_{rr}^{M+1}}{(M+2)! \prod_{v=j\neq r}^{i} (h_{rr} - h_{vv})}, \qquad \text{(F7.2.56)}$$

where (for $h_{rr} \neq h_{vv}$),

$$d_{ij} = \prod_{s=j}^{i-1} h_{ss} \sum_{r=j}^{i} \sum_{k=i-1}^{M} \frac{h_{rr}^{k}}{(k+1)! \prod_{v=j\neq r}^{i} (h_{rr} - h_{vv})}. \qquad \text{(F7.2.57)}$$

The relative errors shown by Eqs. (F7.2.54) and (F7.2.55) are small. However, it appears that lower bounds of d_{ij} in Eqs. (F7.2.56) and (F7.2.57) cannot be reasonably well established, since any r*th* term can have either sign. Also, we note that $R^{M}(d_{ij})$ probably increases as d_{ij} elements are farther from the diagonal. Thus, it may be more appropriate to apply lower bounds of $g(t)_i$ and the absolute error in $g(t)_i$.

F7.2.7.3 Relative Errors in $\underline{G}(t)$ or $r(t)_i$ from Omitting D(H) Series Terms

The matrix D(C), derived from D(H), has an absolute error $E^M(d_{ij})$ plus possible round-off error from its derivation, which is evaluated later. Consider d_{ij} to be elements of D(C). Applying the integral Eq. (F7.2.44), let

$$r(o)_j = n(o)_j \Big/ \sum_{k=1}^{m} n(o)_k \tag{F7.2.58}$$

and

$$r(t)_i = g(t)_i \quad t \sum_{k=1}^{m} n(o)_k = \sum_{j=1}^{m} d_{ij} r(o)_j . \tag{F7.2.59}$$

We know that $E^M(d_{ij}) \leq 5 \times 10^{-16}$. Now we analyze the relative errors $R^M(d_{ij})$ by obtaining a lower limit of all d_{ij} for the *ith* nuclide. Small values of d_{ij} require that the half life of i be much shorter than that of j, or the decay constants $\lambda_i > > \lambda_j$. This is simply the condition that leads to secular equilibrium,

$$\frac{n(t)_i}{n(t)_j} = \frac{|h_{jj}|}{|h_{ii}|} = \frac{\lambda_j}{\lambda_i} . \tag{F7.2.60}$$

If all $n(o)_k$ are zero except $n(o)_j$, the average of $n(t)_i$ exceeds half of that at time t; thus

$$d_{ij} \geq \frac{\lambda_j}{2\lambda_i} . \tag{F7.2.61}$$

Now, the relative error in $r(t)_i$ due to $n(o)_j$ is obtained by dividing Eq. (F7.2.53) by Eq. (F7.2.61). The result is

$$R^M[r(t)_{j \to i}] \leq \frac{\lambda_i}{\lambda_j} 10^{-15} . \tag{F7.2.62}$$

As an extreme case we consider a ratio of decay constants $\lambda_i/\lambda_j = 10^8$, which exceeds any ratio for daughter i and parent j (where $j < i - 1$) of any fission-product chain. This value produces the following error:

$$R^M[r(t)_{j \to i}] \leq 10^{-7} \tag{F7.2.63}$$

However, there are nuclides k (for $i > k > j$) that are not necessarily in secular equilibrium with j, except at large decay times. Thus, we assume

$$n(t)_k \doteq n(t)_j$$

and $\lambda_i >> \lambda_k >> \lambda_j$. Then, dividing absolute error by the magnitudes of n(t) from k and j combined gives

$$R^M[r(t)]_{\substack{k-j \\ j-i}} \doteq \frac{[n(t)_{j-i} + n(t)_{k-i}]10^{-15}}{\dfrac{n(t)_j\lambda_j}{\lambda_i} + \dfrac{n(t)_k\lambda_k}{\lambda_i}} \leq \frac{2\lambda_i}{\lambda_k}10^{-15} << R^M[r(t)]_{j-i} \leq 10^{-7}.$$

This procedure leads to a reduction in the error. Also, the relative errors, $R^M(d_{ij})$, from Eq. (F7.2.56) are less for adjacent nuclides in the chain, as seen in Eq. (F7.2.55). Commonly, the largest relative difference in half-lives is between two adjacent nuclides, in particular that due to a nuclide decaying to the excited state of a nuclide near the valley of stability. Thus, from the above discussion for integral problems within the intended use of the code, the relative error of 10^{-7} in Eq. (F7.2.63) provides a satisfactory bound for $R^M[r(t)]$ or $R^M[d_{ij}]$.

F7.2.7.4 Round-Off Errors in D(H)

Now, consider errors due to truncation or round-off in the process of addition and subtraction by the computer. Each computer subtraction has the general form, for $u > 0$, $v > 0$, and $w > 0$, of

$$u = v - w. \tag{F7.2.64}$$

In order to quantify the round-off error* in u, it is required to derive an upper limit of w/v. First, we evaluate the round-off error in computing D(H) in Eq. (F7.2.52). Let b_{ij}^k be the k*th* process of summing 1 (from I) plus the matrix product from the right in Eq. (F7.2.52); then

$$b_{ii}^k = 1 + \sum_{r=1}^{m} \frac{h_{ir}b_{ri}^{k-1}}{M-k+1} \tag{F7.2.65}$$

for the matrix H of size $m \times m$. The largest w/v is produced from

$$b_{ii}^k \geq 1 - \frac{|h_{ii}|b_{ii}^{k-1}}{2} \geq \frac{7}{8}, \tag{F7.2.66}$$

where, omitting all other $h_{ir}\, b_{rj}^{k-1}$ terms in deriving Eq. (F7.2.66) from Eq. (F7.2.65), bounds $v \geq 1$. Then, since $b_{ii}^{k-1} \leq 1$,

$$\frac{w}{v} \leq \frac{|h_{ii}|}{2} \leq \frac{[H]}{2} \leq \frac{1}{8}. \tag{F7.2.67}$$

Also, for the off-diagonal elements, the following relation was derived:

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*This discussion pertains to round-off of double-precision words on the IBM mainframe (e.g., the IBM 3090). The magnitudes given here, of course, can be different on other computers.

$$b_{ij}^{k} = \frac{h_{ij}b_{jj}^{k-1} + q_{ij}^{k-1} + h_{ii}b_{ij}^{k-1}}{M-k+1} \geq b_{ij}^{k-1}, \qquad \text{(F7.2.68)}$$

where

$$q_{ij}^{k-1} = \sum_{\substack{r=1 \\ j \neq r \neq i}}^{m} h_{ir}\, b_{rj}^{k-1}. \qquad \text{(F7.2.69)}$$

Then, w/v for b_{ij}^{k}, using Eqs. (F7.2.66) and (F7.2.68), becomes

$$\frac{w}{v} \leq \frac{|h_{ii}|b_{ij}^{k-1}}{h_{ij}b_{jj}^{k-1} + q_{ij}^{k-1}} \leq \frac{8[H](h_{ij} + q_{ij}^{k-2})}{7(h_{ij} + q_{ij}^{k-1})} \leq \frac{2}{7}. \qquad \text{(F7.2.70)}$$

The effect of w/v is evaluated later, in the discussion following Eq. (F7.2.85).

F7.2.7.5 Round-Off Errors in D(C), or D(2^nH)

Now, we evaluate the round-off error, or w/v, of elements of D(2^nH), denoted by d_{ij}^{n}. First, for the sake of expediency, various characteristics of these elements which were derived for D(2^nH), either with or without feedback, are listed:

$$1 \geq d_{ij}^{n+1} \geq \frac{1}{2} d_{ij}^{n} \geq 0 \qquad \text{(F7.2.71)}$$

$$0 \geq 2^n h_{ii} d_{ii}^{n} \geq e^{2^n h_{ii}} - 1 \qquad \text{(F7.2.72)}$$

$$d_{ij}^{n} d_{ji}^{n} \leq d_{jj}^{n} d_{ii}^{n}. \qquad \text{(F7.2.73)}$$

The general formula for d_{ij}^{n+1} in the recursion relationship of Eq. (F7.2.50) is

$$d_{ij}^{n+1} = \sum_{r=1}^{m} d_{ir}^{n}(\delta_{rj} + x_{rj}/2) = \sum_{r=1}^{m} d_{ir}^{n} y_{rj}, \qquad \text{(F7.2.74)}$$

where

$$x_{rj} = \sum_{s=1}^{m} 2^n h_{rs}\, d_{sj}^{n} \qquad \text{(F7.2.75)}$$

$$y_{rj} = \delta_{rj} + x_{rj}/2 \tag{F7.2.76}$$

$$\begin{aligned}\delta_{rj} &= 1, \text{ for } r = j \\ &= 0, \text{ for } r \neq j .\end{aligned} \tag{F7.2.77}$$

Consider a feedback term from i to j, or $h_{ji} > 0$. Applying Eq. (F7.2.74) to diagonal elements

$$d_{ii}^{n+1} = d_{ii}^{n} y_{ii} + d_{ij}^{n} y_{ji} = d_{ii}^{n} y_{ii} + 2^{n-1} d_{ij}^{n}(h_{ji} d_{ii}^{n} + h_{jj} d_{ji}^{n}) . \tag{F7.2.78}$$

Also, for the off-diagonal elements

$$d_{ij}^{n+1} = d_{ij}^{n} y_{jj} + d_{ii}^{n} y_{ij} = d_{ij}^{n} y_{jj} + 2^{n-1} d_{ii}(h_{ij} d_{jj}^{n} + h_{ii} d_{ij}^{n}) . \tag{F7.2.79}$$

Only the third terms of Eqs. (F7.2.78) and (F7.2.79) are negative. Using Eqs. (F7.2.73) and (F7.2.72) in deriving w_1, for the first equation

$$w_1 = 2^{n-1}|h_{jj}| d_{ij}^{n} d_{ji}^{n} \leq |2^{n-1} h_{jj} d_{jj}^{n}| d_{ii}^{n} \leq \frac{1}{2} d_{ii}^{n} . \tag{F7.2.80}$$

Also, using Eq. (F7.2.72) we write w_2 for Eq. (F7.2.79)

$$w_2 = |2^{n-1} h_{ii} d_{ii}^{n}| d_{ij}^{n} \leq \frac{1}{2}(1 - e^{2^n h_{ii}}) d_{ij}^{n} \leq \frac{1}{2} d_{ij}^{n} . \tag{F7.2.81}$$

Now, $u_1 \geq d_{ii}^{n}/2$ and $u_2 \geq d_{ij}^{n}/2$ from Eq. (F7.2.71). Thus,

$$u/w \geq 1 , \tag{F7.2.82}$$

or

$$\frac{w}{v} = \frac{w}{w + u} = \frac{1}{1 + u/w} \leq \frac{1}{2} . \tag{F7.2.83}$$

Also, y_{ii} and y_{jj} require evaluations. Using Eqs. (F7.2.76) and (F7.2.75),

$$y_{ii} = 1 + 2^{n-1}(h_{ij} d_{ji}^{n} = |h_{ii}| d_{ii}^{n}) , \tag{F7.2.84}$$

which gives the result for w/v, using Eq. (F7.2.72),

$$\frac{w}{v} \leq |2^{n-1} h_{ii} d_{ii}^{n}| \leq \frac{1}{2} , \tag{F7.2.85}$$

and the same result for y_{jj}. Note that w/v in Eqs. (F7.2.83) and (F7.2.85) are less than ½. Let ΔE be the round-off error for w/v = ½. Then the machine computation of d_{ij}^{n+1} from d_{ij}^{n}, for all i and j, produces less than $2\Delta E$ round-off error. The method of computing D(H) from Eq. (F7.2.52) shows that w/v ratios from each previous calculation of b_{ij}^{k} affect $d(h)_{ij}$ progressively less, by factors of 2/7. Thus, the round-off error of $d(h)_{ij}$ from Eqs. (F7.2.67) and (F7.2.70) for all i and j is less than ΔE. Comparing the calculated d_c^n with the true d_t^n,

$$\begin{aligned} d_c^0 &= d_t^0(1 \pm \Delta E) \\ d_c^n &= (d_t^{n-1} \rightarrow d_t^n)(1 \pm 2\Delta E) \\ d_c^n &\doteq (d_t^{n-2} \rightarrow d_t^n)(1 \pm 4\Delta E) \quad , \end{aligned} \tag{F7.2.86}$$

or

$$d_c^p \doteq d_t^p[1 \pm (2p + 1)\Delta E] . \tag{F7.2.87}$$

The largest IBM mainframe word truncation error for w/v = ½ results from u = 1 and w = 0.5, which, for double precision, conservatively sets ΔE as

$$\Delta E \leq 5 \times 10^{-16} . \tag{F7.2.88}$$

Since 2^{p-2} cannot exceed 10^{76} on the IBM mainframe computers,

$$p < (76)\, \ell n(10)/\ell n(2) + 2 < 255 . \tag{F7.2.89}$$

Using Eqs. (F7.2.88) and (F7.2.89) in Eq. (F7.2.87), we obtain

$$d_c^p = d_t^p(1 \pm 3.1 \times 10^{-13}) . \tag{F7.2.90}$$

The relative uncertainty given by Eq. (F7.2.90) applies to the fission product decay library in ORIGEN-S, which does not have feedback between nuclides in any of the decay chains. While the preceding error analysis generally considered feedback, Eq. (F7.2.83) was derived for only one feedback term in Eqs. (F7.2.78) and (F7.2.79). The inclusion of r feedback terms was analyzed also, and it was determined that the increase in the uncertainty shown in Eq. (F7.2.90) does not exceed r/2.

F7.2.7.6 Round-Off Errors in $\underset{\sim}{G}(t)$ and $\underset{\sim}{N}(t)$

A similar relative error is due to round-off in $r(t)_i$. For some of the nuclides i, however, the truncation of terms in calculating $D^M(H)$ will dominate in the combined error. Even though Eq. (F7.2.90) should apply to $r(t)_1$, and $r(t)_2$, the upper limit to the errors may increase to about 10^{-7} under the conditions discussed for Eqs. (F7.2.60) to (F7.2.63). These limits pertain to the integral results $\underset{\sim}{G}(t)$.

Also, ORIGEN-S produces the regular "instantaneous" results $\underset{\sim}{N}(t)$ from Eq. (F7.2.42). Let Δn_i represent the elements of the matrix product, C D(C) $\underset{\sim}{N}(o)$, in the equation. The effect of multiplying by C is similar to one more application of Eq. (F7.2.75) with $\tilde{h}_{ij}$ replaced with c_{ij}, while the term truncation analysis applied to $n(t)_i$ essentially applies to Δn_i. However, Δn_i represents quantities generated or depleted for the nuclides during time t. When Δn_i is positive, or a negative quantity with a small magnitude in comparison with $n(o)_i$, there is no appreciable round-off problem. However, round-off error becomes significant as $n(o)_i - \Delta n_i$ approaches zero. If $n(t)_i/n(o)_i < 10^{-16}$, the IBM mainframe computer produces for $n(o)_i - \Delta n_i$, either $n(t)_i = 10^{-16}\, n(o)_i$ or $n(t)_i = 0$, due to round-off, producing either **one** or **no** machine bits difference in computing $n(o)_j - \Delta n_j$. It was concluded that quantities decreasing to less than 10^{-12} of their starting value do not have the intended precision of four places. This problem is eliminated in ORIGEN-S by first computing the solution to Eq. (F7.2.39) by applying the model discussed in Sects. F7.2.2 to F7.2.4. Then, all results in which $n(t)_i/n(o)_i \geq 10^{-12}$ are replaced* with the solutions computed by Eq. (F7.2.42).

Note that in applications of the integral model to conditions wherye each d_{ij} requires a very small relative error, the value of M should be properly increased from M = 10. For the usual MeV/fission and reactor fission product problems, this is not considered necessary.

F7.2.8 NEUTRON SOURCE STRENGTHS AND SPECTRA APPLIED TO UO_2 FUEL

The neutron source computed by ORIGEN-S includes that produced from both spontaneous fission and (α,n) reactions of heavy nuclides. The method of computing the spontaneous fission neutron source is independent of the medium containing the fuel. However, (α,n) production varies significantly with the composition of the medium. A discussion pertaining to both the spontaneous fission and the (α,n) data applied to UO_2 fuel is presented here. The next subsection discusses the derivation of the (α,n) source applied to borosilicate glass.

The major part of the neutron source is produced from spontaneous fission of the heavy nuclides. Data required to compute the neutron production rate from this process include the spontaneous fission half-life, the average neutron yield per spontaneous fission, ν_{sf}, and the concentration for each contributing nuclide. Spontaneous fission half-lives for the more significant nuclides are those from the ORIGEN-S card-image actinide nuclear data library (Sect. M6). For several less important nuclides, unmeasured half-lives are taken from Ref. 9. These data were estimated with a correlation between measured data and so-called fissility parameters.[10] The ν_{sf} data are taken from Ref. 9. Measured values are available for 21 nuclides, including the most significant. An equation, derived[9] to compute ν_{sf}, produces values which are within two experimental standard deviations for all except three nuclides. This equation is applied for nuclides that do not have measured data.

A significant neutron source is produced from $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions in the UO_2 and other oxygen compounds of the spent fuel. Thin target cross sections[11] for these reactions and alpha stopping power data were applied to compute neutron yields of the fuel material. Thick target energy-dependent (α,n) yields for $^{238}U^{NAT}O_2$ were computed[11] within estimated accuracies of 10%. These data are applied by ORIGEN-S to the various alpha energies of the actinide nuclides. Although alpha energies are not explicitly given in the ORIGEN-S decay data base (Sect. M6), these data were derived from the same sources as those used to produce the data base. ENDF/B-VI data[12] were used for a large majority of the actinides. Evaluated Nuclear Structure Data File (ENSDF) data[13] were used, if available, for those not in ENDF/B-VI. Then, for the

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*The 10^{-12} is automatically replaced by a value depending on the machine word precision determined by ORIGEN-S for any machine.

remaining actinides (of lesser significance), available data from the *Table of Radioactive Isotopes*[14] were applied. All the yields, energies, and associated data are edited during the execution of the neutron source option if the edit of the actinide library option is requested. These data, which are not contained in the ORIGEN-S library, are supplied in the Block Data COMMON/SPECDT/.

The isotopes ^{242}Cm and ^{244}Cm characteristically produce all except a few percent of the spontaneous fission and (α,n) neutron source in spent PWR fuel over a 10-year decay time. The next largest contribution is usually from the (α,n) reaction of alphas from ^{238}Pu, which is approximately 1 to 2% of the source. Neutron energy spectra of both the spontaneous fission and (α,n) reactions have been determined for the curium isotopes[15,16] and ^{238}Pu.[17] The measured spontaneous fission neutron spectrum of ^{244}Cm was found to be quite similar to that from ^{235}U and ^{252}Cf. Thus, the spectrum for ^{242}Cm was computed[16] from these measurements. The (α,n) neutron spectra were determined by extrapolating the neutron spectrum from Po-α-O source measurements[18] to the alpha energies of ^{242}Cm, ^{244}Cm, and ^{238}Pu. The energy distribution of the spontaneous fission neutron spectrum is computed from the spectra for ^{242}Cm and ^{244} Cm described above, using the calculated concentrations of those two isotopes. This spectrum is then renormalized to include the total neutron source from all spontaneously fissioning isotopes. A similar calculation, using the data for all three isotopes, is performed for the (α,n) neutron spectrum. The spectra are collapsed from the energy group structure of the data to either the group-structure input or that of the SCALE library specified by input. The procedure assumes uniform distribution within each group and simply sums the quantities based upon energy fractions common to both groups in the two group structures. The total neutron source spectrum is then computed as the sum of the spontaneous fission and (α,n) spectra.

F7.2.9 THE (α,n) SOURCE APPLIED TO BOROSILICATE GLASS[19]

In place of UO_2 it may be necessary to apply borosilicate glass containing high-level waste (HLW) as the medium in computing neutron source spectra by ORIGEN-S. Although this requires no change in the method of calculating neutron spectra from spontaneous fission, the (α,n) source derivation is strongly dependent upon the light-element content in the medium containing the α-emitters. For example, the fraction of the neutron source from (α,n) reactions increases from less than 0.1 in typical BWR and PWR spent fuel to more than half of the total neutron source in possible compositions of borosilicate glass containing HLW. The analytical model for treating borosilicate glass mixtures and the source of the (α,n) yield data are presented here.

The neutron production rate from α-emitter i per unit volume, S_i, in neutrons per second, is derived from laboratory-measured (α,n) yields for various light elements j by

$$S_i = N_i \lambda_i Y_{ij}, \qquad \text{(F7.2.91)}$$

where

N_i = number of atoms of isotope i per unit volume,
λ_i = α-decay constant of α-emitter i,
Y_{ij} = (α,n) yield in element j, neutrons per α-emission from i.

Both the total (α,n) yields and the (α,n) yield spectra have been measured for most of the significant light elements.

The (α,n) spectrum produced from combinations of light elements, such as those found in borosilicate glass, may be derived from the (α,n) yields of individual light elements. Since an appropriate weighting

function to be used in combining (α,n) yields of light elements was not considered to be completely established, research was conducted by Pellarin, Matney, and Bibler[20] to compare total mixture (α,n) yields determined experimentally with predicted values from different calculational procedures. The most favorable method produced an (α,n) yield that was 1.6% less than the average measurement of the (α,n) yield of ^{238}Pu in borosilicate glass. This relation for calculating the effective thick target (α,n) yield of a mixture, as derived by West,[21] is a function of the element densities, the decay rates of α-emitters, the α-energy-dependent yields of the light elements, and the α-energy-dependent stopping powers of the elements. Explicitly, the equation for the total (α,n) source strength per unit volume of a mixture, S, which includes all α-emitters i and all isotopes or elements j, can be written as

$$S = \sum_i N_i \lambda_i \left[\sum_j \rho_j P_{ij} Y_{ij} \Big/ \sum_j \rho_j P_{ij} \right], \qquad \text{(F7.2.92)}$$

where

ρ_j = the density (or constant times density) of isotope or element j,
P_{ij} = the α-stopping power of j at α-energy of i.

Note that the yields in Eq. (F7.2.92) are weighted by the product of elemental density and stopping power.

Although the UO_2 model discussed in Sect. F7.2.8 uses spectral data applicable only to oxygen, spectral distributions have been measured for several other light elements. Applying these spectral data, the spectral yields produced in borosilicate glass were computed at the α-energies of ^{238}Pu, ^{241}Am, ^{242}Cm, and ^{244}Cm for the borosilicate glass composition listed in Table F7.2.1.[20] There would not be a large change in the spectral distribution in other similar compositions[22] of borosilicate glass. Finally, the (α,n) neutron source for each energy group per unit volume, s_g, using the four above isotopes k and normalizing to S, is determined by the relation

$$s_g = (S/S') \sum_k N_k \lambda_k Y_k y_{kg} \Big/ \sum_g y_{kg}, \qquad \text{(F7.2.93)}$$

where

S = total (α,n) source strength per unit volume from Eq. (F7.2.92),
S′ = sum of (α,n) source strengths per unit volume of isotopes k,
N_k = number of atoms of isotope k per unit volume,
λ_k = α-decay constants of isotope k,
Y_k = (α,n) yield of isotope k in the mixture, and
y_{kg} = borosilicate glass (α,n) yields of isotope k in group g.

Experimental data for P_{ij}, Y_{ij}, and y_{kg} are required to solve Eqs. (F7.9.92) and (F7.9.93). P_{ij} was not used by ORIGEN-S for the UO_2 model, while Y_{ij} and y_{kg} were applied for ^{17}O and ^{18}O, or, ultimately, UO_2^{11}, only. In the borosilicate glass model, Y_{ij} data for Li, Be, B, F, Mg, Al, Si, and O were taken from measurements by Bair and del Campo.[11] The Y_{ij} data for C were produced experimentally by West and Sherwood.[23] A yield for Na was that reported by Weren and Faulkner.[22]

Table F7.2.1 The borosilicate glass composition used for spectral data

Atomic number	Symbol	Wt %
3	Li[a]	2.18
5	B[a,b]	2.11
8	O[a,b]	46.4
9	F[a,b]	0.061
11	Na[a]	7.65
12	Mg[a,b]	0.49
13	Al[a,b]	2.18
14	Si[a,b]	25.4
17	Cl	0.049
20	Ca	1.08
25	Mn	1.83
26	Fe	8.61
28	Ni	0.70
40	Zr	0.88
82	Pb	0.049
Total		99.669

[a]Elements with total (α,n) yield data in ORIGEN-S.
[b]Elements with spectral data, comprising 77% of the total weight of approximately 85% of the total (α,n) yield.

Neutron energy spectra from (α,n) reactions for the elements B, O, F, Mg, Al, and Si at α-energies of 4, 4.5, 5, and 5.5 MeV were measured by Jacobs and Liskien.[24] These data were interpolated or extrapolated (over a short range) to produce the y_{kg} for ^{238}Pu, ^{241}Am, ^{242}Cm, and ^{242}Cm. Borosilicate glass (α,n) production is strongly dominated by these six light elements used for the spectral distribution. The entire ten elements, for which there are total yield data, are used in determining the normalized (α,n) source, S, applying Eq. (F7.9.92). The problem-dependent densities, ρ_j, of these ten elements in the ORIGEN-S case are applied in computing S.

Stopping powers, P_{ij}, as a function of α-energy and atomic number, Z, are applied from tables produced by Northcliffe and Schilling.[25] These data were given for 12 solid media elements from Be to U and 9 gaseous media elements from H to Rn. Stopping powers of any other element are computed by linear interpolation as a function of Z between data for elements in the same type of medium (solid or gaseous), or extrapolated for elements above U.

The final (α,n) spectral distributions, in relative units, computed from data for B, O, F, Mg, Al, and Si in Eq. (F7.2.93) are listed for ^{238}Pu, ^{241}Am, ^{222}Cm, and ^{244}Cm in Table F7.2.2. These data are incorporated into ORIGEN-S and are normalized to total effective light element (α,n) yield when used with the borosilicated glass option.

Since α-particle range is decreased by increased densities, it is important to describe the problem with the entire borosilicate composition input to the ORIGEN-S case. The input data are discussed in Data Note C, Sect. F7.6.13. (Also, see option number 11 in the 54$ array for applying the borosilicate model.)

Table F7.2.2 (α,n) spectral distributions in borosilicate glass

Neutron energy, MeV	Spectra, relative units ^{238}Pu, ^{241}Am	^{242}Cm	^{244}Cm
0.1	4.40(-1)[a]	5.02(-1)	5.60(-1)
0.2	4.80(-1)	5.44(-1)	6.03(-1)
0.3	4.98(-1)	5.66(-1)	6.30(-1)
0.4	5.27(-1)	5.96(-1)	6.60(-1)
0.5	6.28(-1)	6.85(-1)	7.34(-1)
0.6	7.10(-1)	7.81(-1)	8.42(-1)
0.7	7.66(-1)	8.54(-1)	9.34(-1)
0.8	9.10(-1)	9.89(-1)	1.05
0.9	9.60(-1)	1.08	1.19
1.0	9.19(-1)	1.07	1.22
1.1	9.24(-1)	1.05	1.17
1.2	9.68(-1)	1.10	1.19
1.3	8.97(-1)	1.07	1.25
1.4	9.06(-1)	1.03	1.16
1.5	9.42(-1)	1.06	1.16
1.6	9.85(-1)	1.10	1.20
1.7	1.04	1.15	1.25
1.8	1.15	1.24	1.31
1.9	1.23	1.35	1.43
2.0	1.33	1.44	1.55
2.1	1.51	1.57	1.65
2.2	1.64	1.75	1.81
2.3	1.84	1.91	1.99
2.4	2.04	2.14	2.18
2.5	2.36	2.38	2.43
2.6	2.57	2.73	2.71
2.7	2.79	2.95	3.08
2.8	3.11	3.18	3.32
2.9	3.08	3.43	3.57
3.0	3.11	3.51	3.82
3.1	2.96	3.54	3.91
3.2	2.90	3.40	3.95
3.3	2.68	3.32	3.83
3.4	2.56	3.12	3.73
3.5	2.34	2.96	3.55
3.6	2.15	2.75	3.35
3.7	1.96	2.52	3.15
3.8	1.71	2.32	2.90
3.9	1.58	1.07	2.67
4.0	1.40	1.87	2.43
4.1	1.24	1.69	2.16
4.2	1.14	1.50	1.99
4.3	9.86(-1)	1.36	1.77
4.4	9.27(-1)	1.22	1.58
4.5	8.70(-1)	1.10	1.46
4.6	7.87(-1)	1.03	1.29
4.7	7.33(-1)	9.61(-1)	1.20
4.8	6.64(-1)	8.79(-1)	1.13
4.9	5.02(-1)	8.14(-1)	1.04
5.0	3.75(-1)	7.15(-1)	9.64(-1)
5.1	2.88(-1)	5.44(-1)	8.87(-1)
5.2	2.22(-1)	4.12(-1)	7.55(-1)
5.3	1.01(-1)	3.19(-1)	5.79(-1)
5.4	6.09(-2)	2.41(-1)	4.44(-1)
5.5	4.49(-2)	1.12(-1)	3.47(-1)

Table F7.2.2 (continued)

Neutron energy, MeV	Spectra, relative units ^{238}Pu, ^{241}Am	^{242}Cm	^{244}Cm
5.6	3.82(-2)	6.86(-2)	2.57(-1)
5.7	3.46(-2)	5.12(-2)	1.23(-1)
5.8	2.22(-2)	4.36(-2)	7.59(-2)
5.9	1.86(-2)	3.95(-2)	5.72(-2)
6.0	1.82(-2)	2.68(-2)	4.88(-2)
6.1	1.49(-2)	2.16(-2)	4.42(-2)
6.2	2.56(-3)	2.06(-2)	3.16(-2)
6.3	2.22(-3)	1.77(-2)	2.45(-2)
6.4	2.05(-3)	6.59(-3)	2.29(-2)
6.5	1.94(-3)	2.48(-3)	2.05(-2)
6.6	1.94(-3)	2.31(-3)	1.12(-2)
6.7	1.77(-3)	2.21(-3)	2.72(-3)
6.8	1.71(-3)	2.17(-3)	2.54(-3)
6.9	1.54(-3)	2.00(-3)	2.46(-3)
7.0	1.42(-3)	1.92(-3)	2.39(-3)
7.1	1.37(-3)	1.74(-3)	2.22(-3)
7.2	1.20(-3)	1.62(-3)	2.12(-3)
7.3	1.20(-3)	1.55(-3)	1.93(-3)
7.4	1.14(-3)	1.36(-3)	1.80(-3)
7.5	1.14(-3)	1.36(-3)	1.72(-3)
7.6	1.14(-3)	1.30(-3)	1.52(-3)
7.7	1.14(-3)	1.30(-3)	1.52(-3)
7.8	1.20(-3)	1.30(-3)	1.45(-3)
7.9	1.03(-3)	1.30(-3)	1.45(-3)
8.0	9.11(-4)	1.35(-3)	1.45(-3)
8.1	2.28(-4)	1.20(-3)	1.45(-3)
8.2		1.07(-3)	1.50(-3)
8.3		4.49(-4)	1.38(-3)
8.4		7.01(-5)	1.21(-3)
8.5			7.00(-4)
8.6			1.52(-4)

[a]Read as 4.40×10^{-1}.

F7.3 FEATURES AVAILABLE IN PROGRAM

Main Features of the ORIGEN-S Code

Various features of the code and characteristics of the different types of problems that can be solved are briefly discussed in the following list.

1. An "irradiation" problem is solved using a set of initial nuclide or element concentrations and the "nuclear data library" for a given reactor flux.

2. A "post-irradiation" problem is solved, which may be part of an irradiation subcase or a new subcase.

3. A "decay-only" problem involving no irradiation is solved.

4. A problem is solved using "continuous feed" feature, where the concentrations are enhanced with a continuous rate of feed for given isotopes. This applies to fluid fuel reactors.

5. A problem is solved using "continuous chemical processing" feature, where the concentrations of given elements are depleted by a continuous removal rate through chemical processing.

6. A "continuation" problem is solved where an irradiation or decay subcase begins with the concentrations prevailing at any time specified during the last subcase.

7. Either the same or a different "nuclear data library" may be requested in a continuation subcase. This step allows for different flux spectra to be applied, in order to account for the time dependence of flux within a reactor.

8. A continuation problem is solved using the "batch removal" feature, where given fractions of specified elements are removed through chemical batch processing before calculation continues.

9. A "blending case" is executed, which always will contain several subcases. Different concentrations are used in two or more of the subcases. A given fraction of the material from each of the streams, or subcases, at specified times are added together to form the initial concentrations for subsequent "blended stream" subcases. While different libraries are permitted, there should not be any variation in the lists of nuclides from library to library. Any number of problems not related to the blending option may be solved within the case.

10. The "nuclear data library" input to the code may be in either the "binary" or "card image" mode. Only the "card image" library can be edited. The binary library saves about half the computer time of a ten-time-step problem, can be automatically updated from an XSDRNPM and COUPLE code case, and automatically provides the library sizes which must be user-specified for the "card image" library.

11. There is a division of the isotopes and isomers into three separate groups. The problem computation may be restricted to any combination of the three groups, eliminating needless time or printing in processing an unwanted group. The nuclides of each group (or library) are

a. fuel nuclides and their heavy-metal reaction and decay products plus ^4He,
b. fission products, and
c. light elements common in power reactor coolants, clad, and structural material or in research reactor experimental cells.

12. The user's problem input is in the free-form style, with the numerous conveniences of the FIDO Input System (see Sect. M10).

13. A variety of units is allowed in the input of some of the problem parameters:

a. starting nuclide concentrations may be in grams, gram-atoms, weight ppm, atom ppm, or curies,
b. reactor irradiation may be in terms of thermal flux or power, and
c. time in six different units.

14. The nuclide concentration and associated answers may be converted to a large variety of units for listing. The units available during irradiation depend upon the input units. Possible output units are

a. gram-atoms,
b. grams,
c. weight ppm,
d. atom ppm,
e. atoms/(barn-cm),
f. total delayed gamma source spectra in photons/s, MeV/s, or MeV/Ws of burnup,
g. fraction of total neutron absorption rates,
h. total neutron production,
i. total neutron absorption, and
j. infinite medium neutron multiplication constant, k_∞.

Output units available during the decay period are

a. gram-atoms,
b. grams,
c. curies,
d. thermal power afterheat in watts,
e. gamma power afterheat in watts,
f. cubic meters of air containing nuclide quantity to produce density equal to Radiation Concentration Guide (RCG) limit for air (Sect. M6),
g. cubic meters of water to equal RCG limit for water (Sect. M6),
h. neutron sources from (α,n) reaction in either UO_2[11] or borosilicate glass,[19]
i. neutron sources from spontaneous fission,
j. total gamma source spectra[26,27] in photons/s, MeV/s, or MeV/Ws of burnup, and
k. neutron source spectra[27,28,19] from (α,n) plus spontaneous fission in neutrons/s.

15. In general, only tables in the units specified are listed and these are divided into only those groups (see item 11) selected. These may be listed by either nuclide or element. Quantities below the cutoff for the unit may be deleted. The cutoffs may be given either in terms of the units or as percentages of the unit totals.

16. The gamma photon release rate spectra may be computed using three different photon constant data bases. The most recent data base has improved quality and can be periodically updated (Sect. M6).

17. An energy group structure or the unit number of a SCALE library with the desired group structure may be input for producing gamma source spectra. The sources may be saved as an output file. The sources from the three libraries or groups (see item 11) may be combined.

18. The photon data base in the "nuclear data library" may be updated from improved constants in the other data bases.

19. Principal photon sources in photons/s, by nuclide, may be listed by energy group from the fission products. The percentage of source used to select nuclides may be controlled by input.

20. A computation model[8] has been applied to the fission products which produces both time-dependent decay concentrations and their time integral over the time step.

21. Starting concentrations may be saved as an output file. Also the totals of many of the tables listed may be saved.

22. All concentrations (g-atoms) and source spectra at any or all time steps may be saved on a binary data set. A restart feature allows a case to start with any of the saved values.

23. The core storage required for executing the program automatically expands and contracts to fit the problem. Array storage size may be input.

24. All input data, normally read as "card-image" records, may be input from a binary written interface—allowing easy recycle into and out of the program.

25. The removable thermal energy per fission, which is dependent on time and concentration, is computed for each time step by default. Also, an input option allows users to select 200 MeV/fission.

26. A table of contents is located at the end of each run.

27. Substantially improved data have been applied in calculating neutron sources, along with new models for (α,n) reactions and the energy-dependent neutron spectra in both UO_2 and borosilicate glass (Sects. F7.2.8 and F7.2.9).

28. ORIGEN-S automatically determines the machine precision and, subsequently, the maximum size norm of the A-matrix [Eq. (F7.2.11)] used in extracting elements from the matrix. Thus, from the standpoint of selecting the Bateman equation model for the proper nuclides, ORIGEN-S is machine independent.

29. Concentrations, neutron and photon emission rates, and neutron and photon spectra that are computed by ORIGEN-S may be saved and plotted (in a variety of units) by the PLORIGEN code (see Sect. F15).

A version of ORIGEN-S was modified by Williams[29] to perform the "adjoint" computation. The code, named ORIGEN-A, is used for sensitivity analyses, determining the importance of the uncertainty of one nuclide's cross section upon the uncertainty in the ORIGEN-S model computation of the concentration of another nuclide.

F7.4 RANGE OF APPLICABILITY AND DISCUSSION OF UNCERTAINTY

Two main sources of uncertainty are found in the results computed by ORIGEN-S. One of these sources arises from the nature of the techniques for removing transition matrix elements that have absolute magnitudes greater than the prescribed matrix norm. The other deviation in the computed concentrations is from the uncertainties in the data base (i.e., from cross sections, decay constants, and branching ratios).

The computation of discharged material inventories from reactors is probably the primary function of ORIGEN-S. This function includes predictions of various properties and radiation sources during cooling periods of the reactor discharge, both in storage or within chemical processing stages. Therefore, discussion is directed towards the effect of uncertainties in results with regard to these intended applications.

In discussing the first source of uncertainty, we recall the theory in Sects. F7.2.2 and F7.2.3. In the chain A → B → C where A and C are long-lived nuclides and B is short-lived or the "queue of short-lived nuclides," B is removed from the chain and the reduced matrix contains an adjusted value in the element for A. Also, the "beginning-of-interval" concentration of C is augmented to properly reflect its increase due to B. The assumptions applied in the algorithm produce only approximately correct results. However, calculations from this method asymptotically approach the true values if smaller time intervals are used for the same time period, or as the computation progresses over longer time periods. In cases involving an irradiation period of one month to three years for a LWR, it becomes necessary, or more appropriate, to apply at least ten time steps to the period. This method usually applies properly to thermal flux levels of 10^{13} to 10^{14} neutrons per cm^2-s. Such values of the flux level should not be regarded exactly as the upper limit for ten time steps. If higher flux levels are applied, the users should compare answers of cases in which the number of time steps are doubled, or more, and determine for themselves the condition for computing acceptable accuracies. Usually the uncertainties of the major isotopes are of primary importance, while there is less significance in others that are produced in trace quantities. A "sense of proportion" should be applied in establishing the proper setup of the problem. Thus, the model uncertainty should be compared with that produced from the data base, as discussed below. Early in the decay period the isotopic distribution tends to have a more rapid decrease in some of the isotopes that had reached a generation-decay equilibrium during irradiation. Later the distribution is dominated with the asymptotic buildup of stable and long-lived nuclides. Thus, the accuracy in the calculated isotopic distribution increases with decay time. It has been found to be effective to start the decay period with a week or month time step and increase each interval size by no more than a factor of 3. Users should be aware, also, that they may set the lower limit of the number of terms used in the series of Eq. (F7.2.5) by input for the variable NTERM (Sect. F7.6.10). If results do not appear to be correct for high flux, it may be necessary to increase NTERM.

Probably the largest inaccuracy in the results for most nuclides stems from uncertainties in the cross-section data. Three factors contribute to this uncertainty: (1) the standard deviations in the measurements of the cross sections; (2) computational approximations in the processing of cross sections for the representative conditions of the reactor; and (3) the fact that the time linearity assumption of the ORIGEN-S model is not completely valid. The experimental data are continually being improved. In addition to the initial libraries by Bell,[1] there have been various improved libraries produced at ORNL. The SAS2 control module in the SCALE system applies a model that simulates reactor conditions in producing cross sections and allows a large number of time-dependent libraries to be used by ORIGEN-S, all in a single computer job. The cross-section uncertainty due to factors (1) and (2) clearly dominates the error source in comparison to that from the model in factor (3) for typical reactor cases.

A large quantity of data other than cross sections is contained in the "nuclear data libraries." Considerations pertinent to this data are as follows:

1. The calculation can require a large amount of fission product yield data. The yields differ for each fissile isotope. Also, yields are available to ORIGEN-S for only five fissile nuclides per reactor library, as seen in the table is Sect. F7.6.3. The user should be aware that **no** fission products will be contributed by **other** fissile nuclides. Also, for a flux exposure of a small fraction of a second, the fission product energy release computed during the first few seconds of cooling is significantly smaller than the experimentally observed value. This may reflect difficulties in measuring yields of short-lived nuclides that are near the beginning of the chain.

2. The gamma source spectra have been greatly improved from that produced by the initial libraries, first by applying the ENDF/B-IV data, and later by applying the Master Photon Library.[30]

3. Caution is required in decay cases starting with a single nuclide A, in the chain discussed above, since the decay constant ratios may be such that daughters of C are overpredicted.

4. Since ORIGEN-S is a "point model" code, the computed k-infinities can be much less accurate than those from many neutronics codes. A cell-weighted cross-section library for a complete reactor core is required to produce an accurate value of k_∞. The relative changes in their time-dependent values can be useful but should be interpreted properly.

F7.5 PROGRAM STRUCTURE—DESCRIPTION AND INTERRELATIONSHIP OF MAJOR SUBROUTINES

Routine Name: ORIGNS

Calling Routine: Program Entry Routine

Routines Called: MESAGE, OPENOR, ALOCAT (ORDRVR), INQOPN

Routine Functions: Entry to program when applied as "stand alone" code. The I/O data set storage buffers are assigned by OPENOR before calling ORDRVR via ALOCAT.

OPENOR — Data set unit numbers are set to default values or they are read (by 0$ array data). All data sets are opened.

INQOPN — If a data set found unopened through an INQUIRE, calls OPNFIL (in SCALE library) to open it.

Routine Name: O0O004

Calling Routine: Program Entry Point

Routines Called: MESAGE, OPENOR, ALOCAT (ORDRVR)

Routine Functions: Entry to program from SCALE Driver as specified by a SCALE Control Module. Sets flag denoting that case input is supplied by binary interface data set produced by a SCALE Control Module. Other functions are same as ORIGNS.

Routine Name: ORDRVR

Calling Routines: ORIGNS and O0O004 via ALOCAT

Routines Called: CLOSEO, FLXDIM, ORIGEN (XORIGN), NUDATA, and MCHINP

Routine Functions: Its main purpose is the calling of the three major branches which perform: reading and storing the case or subcase data input (FLXDIM); reading and processing the library data input (NUDATA); and the problem computation (ORIGEN).

ALOCAT — Routine for determining storage area used for array variable storage.

CLOSEO — Rewinds some of the I/O units.

MCHINP — Computes machine word precision.

ORIGEN — Interface to XORIGN (Note: Most of the major subroutines are called by way of an interface subroutine, in which the base address pointers of all arrays are set. The name of the major subroutine is that of the interface, prefaced with "X," with the right-most vowel deleted when there are six characters in the interface name.)

Routine Name: XORIGN

Calling Routine: ORDRVR via ORIGEN

Routines Called: FLUX0, DECAY, EQUIL, TERM, NEUT, NTGRAL, GAMLIN, GAMMA, OUTPUT, XOUTDX

Routine Functions: XORIGN controls the major flow of execution paths in computing the solutions to the specified problems. The array XZERO is initialized with the initial concentration $\underset{\sim}{N}$, as denoted in the Eq. (F7.2.20) to be solved. The starting concentrations of each time step are moved to array XTEMP. The computed results, $\underset{\sim}{N}(t)$, are returned to XORIGN in the matrix array XNEW. Major output routines are called. The numerous options are controlled by XORIGN. The control variables and briefly stated options are NREAD, integral model; NOBLND, KT, stream blending; MMN vs M, flux exposure vs decay only; MSUB, continuation subcase; NXCMP, restart case; MFEED, continuous feed; JOPT(1), neutron absorption fraction; LNGAM, special gamma spectra; NGO, preparation for next subcase.

Routine Name: XFLUX0

Calling Routine: XORIGN via FLUX0

Routines Called: POWERF

Routine Functions: Given an input value for the specific power, XFLUXO solves for the average flux over the time interval by using Eq. (F7.2.30) and energy per fission data. Given an input value for the neutron flux, XFLUXO solves for the specific power by Eq. (F7.2.32). Having obtained a value for the neutron flux, XFLUXO generates the first-order rate constants for neutron-induced reactions. Then the diagonal matrix element is formed for each nuclide by combining the disintegration constant, the rate constant for neutron-induced reactions, and the rate constant for removal processes that are proportional to the nuclide concentration. The diagonal matrix elements are stored in the D array.

POWERF — Computes the concentration-dependent ratio of energy (MeV) per fission to 200 MeV/fission, if the default option is requested.

Routine Name: XDECAY

Calling Routine: XORIGN via DECAY

Routines Called: None

Routine Functions: XDECAY determines which nuclides have half-lives that are less than 10% of the time interval and solves for their concentrations using the Bateman solution, Eq. (F7.2.15). The end-of-interval concentrations are stored in the array XNEW. XDECAY also augments the concentrations of long-lived daughter products and stores the augmented beginning-of-interval concentrations in the array XTEMP.

Routine Name: XTERM

Calling Routine: XORIGN via TERM

Routines Called: MATREX

Routine Functions: XTERM forms the reduced coefficient matrix such that it satisfies the criteria inherent in Eq. (F7.2.11). This involves the elimination of the transitions involving those nuclides with short half-lives, the computation of matrix elements required in this elimination, and the use of the augmented beginning-of-interval concentrations calculated in XDECAY. XTERM goes on to solve the reduced system of equations by the matrix exponential method. This method uses the recursion relation, Eqs. (F7.2.9) or (F7.2.24), to obtain the solution, Eq. (F7.2.23). The solution is contained in the array XNEW.

MATREX — Performs the matrix exponential method recursion computation, after arrays initialized in XTERM.

Routine Name: XEQUIL

Calling Routine: XORIGN via EQUIL

Routines Called: None

Routine Functions: XEQUIL sets short-lived daughters of long-lived precursors into secular equilibrium with their parents. This results in the set of equations, Eq. (F7.2.18), that is solved through the Gauss-Seidel iterative technique. The iterative sequence for the concentrations is given in Eq. (F7.2.19). The results are stored in the array XNEW.

Routine Name: FLXDIM

Calling Routine: ORDRVR

Routines Called: PHOLIB, FIDAS, QOREAD, TRN, PAGE, NIMAXS, SCALEN, XOUTPR, WABUND, WI, FLEX1, FLEX2, FLEX3, FLXDI1, FLXDI2, FLXDI3, FLXDI4, INQOPN

Routine Functions: The main purpose performed is to flexibly (variably) dimension all of the code (permitting storage to expand or contract to fit the specified problem). (NTGRAL, GAMLIN, and SPECTR also flexibly dimension arrays for specific options.) FLXDIM alternately reads input problem data and constructs array pointers. Permanent arrays are placed first in the allocated storage and are followed with pointers that effectively overlay the temporarily used arrays. Array sizes are determined by one of four methods: initial defaults, parameters in input, exact sizes in header record of binary-mode libraries, or exact sizes returned from XNUDAT after library data processing. Also, all defaults of input data are set. Other minor data preparation is performed. Error statements are printed, program stops are included, and arrays of important control parameters are briefly printed. Smaller program size is achieved by delegating part of the functions of FLXDIM to routines named FLXDIi, where i = 1, 4. FLXDIM documents array pointer numbers for each array name in comment statements.

FIDAS — Using FFREAD, reads FIDO-SYSTEM card input data. Arrays automatically stored at proper pointer by making position of pointer correspond to array number specified in the input description.

QOREAD — Reads data directly from binary interface produced by SCALE control module.

TRN — Transposes chemical processing input data matrix.

PAGE — Prints Library Edit "prologue" page of references.

NIMAXS — Computes correct size of input variable N1MAX (in 81$ array) for options not requiring it to be input.

SCALEN — Produces data set containing requested concentration results for reading by other codes or a restart option in ORIGEN-S. Calls GBOUND to produce correct photon energy boundaries for PLORIGEN code.

XOUTPR — Prints table of contents of subcases.

WABUND — Computes natural abundances of isotopes of elements if input units are grams instead of gram-atoms.

WI (and WJ) — Prints short edit (a few lines) of final control parameter arrays.

FLEXi — i = 1,3 – Perform minor storage movement of arrays.

FLXDIi — i = 1,4 – Perform part of the functions of FLXDIM.

Routine Name: XNUDAT

Calling Routine: ORDRVR via NUDATA

Routines Called: HALF, MORDAT, NOAH, NUCERR, WABUND

Routine Functions: XNUDAT uses the nuclear data from ORIGEN "card image" libraries to construct a portion of the transition matrix A. The nonzero, off-diagonal terms of A are stored in the array A with three vectors of integer information being developed to be used in locating the matrix elements. It stores the total capture and fission cross sections and decay constants in TOCAP, FISS, and DIS arrays, respectively. Edits, if requested.

HALF	Returns decay constant from half-life.
MORDAT	User-supplied routine, if desired, for obtaining user's library data.
NOAH	Converts Nuclide ID Number (Sect. F7.6.7) to chemical symbol, mass number, and either metastable symbol "M" or blank.
NUCERR	Prints statement giving library size input and "Correction Attempted" when the size input or the default was less than actual size. Then library input is restarted, and case continues.
WABUND	Computes natural abundances of isotopes of elements, if input unit is grams instead of gram-atoms, called from XNUDAT for card image library processing.

Routine Name: XPHOLB

Calling Routine: FLXDIM via PHOLIB

Routines Called: NOAH

Routine Functions: XPHOLB reads the photon production constants. The original ORIGEN library has 12-energy-group constants for the fission products and structural materials and 18 group constants for the actinides and their daughters. However, the user may select other photon group structures from those available in the photon libraries in the SCALE system data base. In this instance, ORIGEN-S may be applied, with proper option signified by control variable LNGAM, to update the photon library and alter the energy group structure. Edits, if requested.

NOAH	Converts Nuclide ID Number (Sect. F7.6.7) to chemical symbol, mass number, and either metastable symbol "M" or blank.

Routine Name: XBINLB

Calling Routine: ORDRVR via NUDATA

Routines Called: None

Routine Functions: Reads and stores part of an ORIGEN-S "binary" library. In this instance, all of the arrays constructed in XNUDAT are read directly for the reactor pertaining to the binary library data set. This includes the transition matrix $\underset{\sim}{A}$, which has already been computed from specific weight factors. Using the binary library saves CPU time.

Routine Name: XBINPH

Calling Routine: FLXDIM via PHOLIB

Routines Called: None

Routine Function: Reads and stores all of the photon production constants from an ORIGEN-S "binary" library, similar to XPHOLB.

Routine Name: XOUTPT

Calling Routine: XORIGN via OUTPUT

Routines Called: LIMITS, XOUT1, XOUT2, XOUT3, XOUT4

Routine Function: Prints tables listing results for different properties, or units, of irradiated or decayed material. Tables are listed either by nuclides or by elements. Totals are shown. Concentrations at the input time intervals, computed earlier in ORIGEN-S, are available in the array XNEW. These results are converted to the units of a particular table prior to printing each line. Values at time interval MSTAR are compared with the input array CUTOFF for deleting lines the user considers irrelevant. Separate tables are printed for the three libraries. For tables pertaining to the irradiation period, the user may request all tables listed by nuclides and/or those listed by elements; and, also, the user may delete or request these tables for each of the three libraries. For the decay period, the nuclide, element, or pair of summary tables may be separately requested or deleted.

LIMITS	Sets "DO-LOOP" limits of each library
XOUTi	i = 1,4 – Perform parts of the functions of XOUTPT.

Routine Name: XGAMMA

Calling Routine: XORIGN via GAMMA

Routines Called: NOAH

Routine Function: Prints tables listing photon release rate spectra and neutron production rates. It uses computed concentrations in the array XNEW, the nuclide photon per disintegration spectra that were written on NDISK by XPHOLB or XBINPH, the (α,n) yield rates (per gram-atom) in library-processed array ALPHAN, and the spontaneous fission neutron production rates (per gram-atom) in library-processed array SPONF. XGAMMA also prints principal fission product sources for each nuclide that contributes as much as 5% (or fraction read in CUT) of the total energy of the group for the time interval MSTAR.

NOAH — Converts Nuclide ID Numbers (Sect. F7.6.7) to chemical symbols, mass number, and either metastable symbol "M" or blank.

Routine Name: XNEUT

Calling Routine: XORIGN via NEUT

Routines Called: SORTPN

Routine Function: Computes k-infinities, neutron productions and absorptions (total), actinide absorptions, non-actinide absorption fractions (total), and fraction of total absorption rates for individual nuclides, if requested by JOPT(1) $\neq$ 0 in 54$ array. The k-infinities are computed by a simplified model, which assumes cell-weighted cross sections for all materials of an infinite lattice pin geometry. Arrays XNEW, FLUX, TOCAPZ, and GENNEU contain data of concentrations, flux, σ_c, and φ, respectively.

SORTPN — Given the absorption fractions in array RERATE and ascending order integers in array JPOINT, SORTPN sorts the integers to point to the ascending order of the absorption fractions. Then, XNEUT prints the nuclides in the descending order of their absorption fractions of the last time step.

Routine Name: INTSET

Calling Routine: XORIGN via NTGRAL

Routines Called: REORD, SORTP

Routine Function: Recasts the transition matrix A into each of the submatrices formed from fission product nuclides of identical mass numbers. Each submatrix is written on data set |NVERT| specified in the 3$ array. INTSET is called if NVERT $<$ 0. The code

uses a previously produced submatrix data set if NVERT > 0. These matrices are used by XNTGRL when invoking the integral option.

REORD — Remakes Nuclide ID Numbers to start on left with the mass number in place of the atomic number (see Sect. F7.6.7).

SORTP — Sorts array NUCL into ascending order. Reorders integers of array NUX to point to the corresponding order of data in arrays DIS, NON0, and KD. This algorithm allows procedure in INTSET to use sorted data without actually reordering the arrays. (SORTP and SORTPN are identical except that they sort integer and real numbers, respectively.)

Routine Name: XNTGRL

Calling Routine: XORIGN via NTGRAL

Routines Called: NVRP, NVREX, NVRDC, NVRDIF

Routine Function: Controls the computation of integration of quantities over the time step intervals for the decay period of fission products only. The model uses the Volterra multiplicative method applied by Lee.[8] Submatrices produced by INTSET are read and stored in array C. The solutions by Eqs. (F7.2.42) and (F7.2.44) are obtained mostly from subroutines and stored in XNEW and YNEW, respectively.

NVRP — Computes p + 1, [H] and H from Eqs. (F7.2.46), (F7.2.51), and (F7.2.45) as NP, HNORM and array H, respectively.

NVREX — Computes D(H) in array D from Eq. (F7.2.48).

NVRDC — Computes D(C) in array D, applying the recursion relationship in Eq. (F7.2.50) for NP times.

NVRDIF — Computes $D(C)\underset{\sim}{N}(0)$ in array XINT as part of Eq. (F7.2.44) and $CD(C)\underset{\sim}{N}(0)$ in array DIFF as part of Eq. (F7.2.42). Final $\underset{\sim}{G}(t)$ and $\underset{\sim}{N}(t)$, then, are obtained in XNTGRL.

Routine Name: GAMLIN

Calling Routine: XORIGN

Routines Called: PHONEW, GAMNEW

Routine Function: Calls subroutines that determine the photon energy spectra using either the Master Photon Library, the ENDF/B file, the ORIGEN-S Input Library, or the special actinide data. GAMLIN and SPECTR set variable array pointers.

PHONEW — Sets triggers denoting which libraries are to be processed in determining the spectra and prints the type of input library and the type of spectra to be computed. ISERCH is called to produce both the array NPT, which points to the next nuclide index, and the array NZ, which contains Z pointers to NPT at positions indexed by IZ = atomic number. Sets M = 1 if LNGAM > 3.

GAMNEW — Calculates a spectrum for each time step requested by the user. GAMNEW calls SPECTR for each selected time step.

Routine Name: SPECTR

Calling Routine: GAMNEW

Routines Called: GSMSET, RITACT, RITFPR

Routine Function: Decides on type of library requested from control variable LNGAM and calls proper subroutine. Calls GSMSET for data from Master Photon Library or ORIGEN-S Library, RITFPR for data from the ENDF/B file, and RITACT for special actinide data. SPECTRA also sets array pointers not set by GAMLIN.

RITACT — Produces spectra for ^{239}U and ^{239}Np from special library of ENDF/B-V processed γ-line data. RITACT calls only DPRSEC (see RITFPR).

Routine Name: GSMSET

Calling Routine: SPECTR

Routines Called: GSMAST

Routine Function: Prepares data from input or defaults (i.e., energy group structure) to that needed by GSMAST for producing a problem photon spectrum or library. The magnitude of each group in the spectrum returned by GSMAST is increased by the ratio of total gamma energy of all nuclides in the ORIGEN-S library requested to the total of only those for which spectral constants were available. This normalization is not performed if the user sets M(K) < 0 in the 82$ input array. When a new binary library is requested by LNGAM > 11, GSMSET updates the energy group structure and sets the new library record position on unit MPHOT (NXTR) to the proper record for the updated photon constants produced in GSMAST. When the ORIGEN-S input library is applied in computing spectra, it sets the record position on unit NDISK to the record to be read by GSMAST. It converts problem spectra to MeV energy units and prints both types of spectra. For NPUN > 0 it writes on NPUN the group structure and the energy spectrum in ascending order and the photon spectrum, in both ascending and descending energy order, in FORMAT (1P5E12.4, 12X, "units").

Routine Name: GSMAST

Calling Routine: GAMSET

Routines Called: None

Routine Function: Reads the Master Photon Library, either as binary or BCD, if requested. Photons/disintegration constants (RI at energy RE) are binned into the proper energy group of average energy EAV. GSMAST converts RI to RI*EAV/RE in order to conserve energy. When the line energy is within 3% of the group's energy range from either boundary, RI/2 is binned in the same manner into the two adjacent groups. This avoids a high or low bias for continuous data recorded at points near group boundaries. All final library arrays (RINT) are added to data on the unit NDISK, to be used in other time steps of the subcase. If an ORIGEN-S library is requested, the array is read directly from the first three records on unit NDISK. When creating new ORIGEN-S libraries, the library array RINT produced, as discussed above, can be used to update either a binary or BCD library. Also the group structure and format (if BCD mode) are written. When computing spectra, the products XNEW*DIS*RINT with proper nuclide and group indexing are summed in spectrum array DBIN.

Routine Name: RITFPR

Calling Routine: SPECTR

Routines Called: NSERCH, DPRSEC, LIBPUN, CONTIN, LIST, SKPSCT

Routine Function: Main function is the production of a photon spectrum of fission products using the ENDF/B-IV file as the data base. RITFPR reads the title card of the spectrum. It obtains library photon group constants for a nuclide, and the disintegrations per second of the nuclide and sums their product in the proper group of array DBIN. It converts the final photon spectrum to units of MeV/s or MeV/fission and prints both spectra. Internal conversion electron data are converted to the proper x-ray energy pertaining to the proper K or L shell and binned. This routine calls LIBPUN for producing libraries using ENDF/B data.

NSERCH — Searches NZ and NPT for index of current nuclide from ENDF/B file.

DPRSEC — Computes disintegrations per second of current nuclide.

LIBPUN — Writes either on unit NPUN the BCD library, or on unit MPHOT (NXTR) the binary library, which is produced from the ENDF/B data base.

CONTIN, LIST and SKPSCT – Special standard ENDF/B-IV file processing routines, for purposes such as reading the next nuclide data list and skipping part of the data in a proper manner.

Routine Name: SRCALC

Calling Routines: XORIGN via NSPEC

Routines Called: CLPS, YIELDN, SUBSTI, NSPBOR, ENRMEV, SMALSR, WRNEUT, TOTALN, NOAH

Routine Function: NSPEC sets array pointers, prepares the arrays of ORIGEN-S spent fuel concentrations, obtains more complete spontaneous fission decay constants in SUBSTI, and calls SRCALC for the remainder of the neutron-source-spectra computation for UO_2. The SRCALC coding follows the procedure described above (Sect. F7.2.8). Source strengths from major isotopes and the total are obtained for spontaneous fission first, and then for (α,n) reactions, computed by a quadratic data fit in YIELDN. The fine-group spectra are made in the arrays FINESP and FINEAL for the above interactions, respectively, by weighting according to source magnitude. They are collapsed to the energy-group-structure input or that of the SCALE library in CLPS and added together for the final neutron source spectrum. SMALSR is called from SRCALC when the neutron source is zero or the ^{244}Cm is less than approximately 10^{-19} gram-atoms to ensure small and zero neutron sources are correct. NSPEC calls ENRMEV to convert group energy boundaries to MeV from eV and to eV from MeV. Also, NSPEC calls TRANF to move concentration to an array of one dimension and WRNEUT for printing neutron spectra. TOTALN, called from WRNEUT, computes the sums of array vectors for the printout. If JOPT(11) = 1, NSPEC calls NSPBOR for the (α,n) model in borosilicate glass.

Routine Name: SRCBOR

Calling Routine: NSPEC via NSPBOR

Routines Called: CLPS, YIEBOR, SUBSTI, ENRMEV, SMALSR, WRNEUT, TOTALN, NOAH

Routine Function: NSPBOR and SRCBOR have functions for computing neutron source emission and spectra for the (α,n) production in borosilicate glass that correspond to similar functions by NSPEC and SRCALC for same type of calculation applied to UO_2. NSPBOR sets array pointers, gets concentrations in proper array by calling TRANF, obtains spontaneous fission data in SUBSTI, and calls YIEBOR and SRCBOR for the neutron source spectra computed for the borosilicate glass model [JOPT(11)=1]. The theory and equations of the model are described in Sect. F7.2.9. YIEBOR computes the (α,n) emission rate for each α-emitter at each time step and the initial time. These are stored in the YA array. SRCBOR obtains source strengths for major isotopes and the total for spontaneous fission and (α,n) reactions, using the YA array vector sent by NSPBOR. The fine group spectra are made in arrays FINESP and FINEAL for the above interactions, respectively, by weighting according to source magnitude. Finally, the spectra are collapsed in CLPS to the energy group

structure specified and added together for the total neutron source spectrum. The auxiliary routines ENRMEV, SMALSR, WRNEUT, and TOTALN have uses identical to those in NSPEC and SRCALC.

F7.6 ORIGEN-S INPUT DESCRIPTION

The ORIGEN-S code determines quantities or activities of elements or isotopes that are present after various time durations. These calculations may consider only the effect of radioactive decay or the effect of both irradiation and decay.

General comments of importance and the interpretation of certain words or phrases are presented first. Reference to these somewhat arbitrary definitions may enhance some of the explanations in the input description.

The user should have read, at least, the introduction and features sections (F7.1 and F7.3) prior to reading this section.

As a "time-and-effort-saving" alternative to reading and learning this input description, the user may prepare ORIGEN-S case input using the ORIGNATE PC code. ORIGNATE can produce a case input file (which may include mainframe JCL) by assisting the user with pull-down menus, screens having self-contained procedural "prompts," and optional "help" information boxes for every data entry. These techniques sharply reduced input preparation time, eliminate the necessity of reading the more complicated details, and appear to be a significantly positive response to the more impatient user. The input description given here may then be used either as a reference or for special cases or changes to cases that require a more complex set of options. The ORIGNATE User's Manual is included as Appendix F7.A in this section of the SCALE document.

F7.6.1 THE INPUT STRUCTURE

It may be useful to have a general understanding of the structure of the input requirements. A brief outline follows:

I. Library request parameters and options
   - A. Data set unit numbers
   - B. Sizes and types of libraries
   - C. Edit controls
   - D. Optional additions to libraries

II. Data describing problem submitted
   - A. General control flags and options
   - B. Sizes of data arrays and other parameters
   - C. Arrays of data needed in describing problem
   - D. Controls for selecting types of tables printed

The data are divided into six data blocks. The input data in Part I are contained in four of the blocks, with the most frequently used data in Data Block 2. The input outlined in Part II, A and B, is entered into Data Block 5, and the input in Part II, C and D, which is usually the largest part of the data, is entered into Data Block 6.

A variety of options may be requested in Data Block 5. While the arrays required for all options are encompassed in the Data Block 6 description, only that data pertaining to the problem requested needs to be entered.

F7.6.2 COMMENT ON CONDENSED AND DETAILED INPUT

A large variety of options and features are allowed in the ORIGEN-S code. Since the need to describe input in sufficient detail required a somewhat long input description, a more condensed version of the input description was written, also. Experienced users may prefer the shorter version. Also, when using the code for the first time, the user may wish to scan the condensed version first, in order to determine the general nature of the input required. The condensed input description is presented first.

F7.6.3 NUCLEAR DATA LIBRARIES

The major part of the total input to ORIGEN-S is supplied by data libraries. Previous data used by ORIGEN and, initially, by ORIGEN-S have been significantly updated in the ORIGEN-S data libraries, which are described in Sect. M6. Even though small libraries have been compiled for special cases, libraries have been produced that contain almost 1,700 nuclide positions. Isomers of isotopes may be included in the list of nuclides.

The library is divided into three libraries for various reasons:

1. Light Elements and Structural Materials (Cladding)
2. Actinide and Heavy Elements (Fuel)
3. Fission Products (From Specific Fissile Isotopes)

Most of the nuclides are different in the three libraries, although it is not an essential requirement. Some of the fission products can appear in the Light-Element Library; and, it may be desired for helium to appear with the actinides, since it results from alpha decay. The printed output is separated into tables for each of the three libraries (sometimes referred to as Library 1, 2, or 3).

Input libraries to ORIGEN-S may be written in two different modes: card image (formatted) or binary (unformatted). A "card image library" is contained in two data sets, consisting of data for four different reactors. It contains three-group cross sections (or two groups per reaction). Three weight factors, applied equally to all nuclides, are required in the data input. The factors may be altered to approximately reflect spectral shifts between different sets of conditions for a type of reactor. The three "nuclear data" library segments (cross sections, etc.) are in the first position and followed by corresponding "photon spectra" segments. The six library segments are contained in a single data set in which a blank card or several blank cards separate each library. All of the decay characteristics data are contained in another data set. A "binary library" is contained in a data set, with data for a single reactor and given sets of conditions at one or more fuel-burnup intervals or operating-time periods. Binary libraries may be significantly improved with data from multigroup cross sections produced in the execution of the XSDRNPM-S code for a case describing the reactor conditions in detail. The binary libraries are easily updated with the improved data (correctly flux weighted) by using the COUPLE code. The three weight factors are computed in the COUPLE code, also, and applied to nuclides for which multigroup cross sections were not requested. A binary library pertaining to any LWR assembly may be produced by a SAS2 case (see Sect. S2).

Fission product yields are included in the libraries for fissile isotopes that appear to be the most significant. The card image libraries contain five isotopes with these yields for each reactor library. These are given in Table F7.6.1. The yields for those not footnoted are from thermal-neutron-induced fissions.

Table F7.6.1 Fissile isotopes with fission product yields

Reactor	Isotopes (in the order of yield data in library)				
HTGR	^{233}U	^{235}U	$^{232}Th^a$	$^{238}U^a$	^{239}Pu
LWR	^{233}U	^{235}U	^{241}Pu	$^{238}U^a$	^{239}Pu
LMFBR	$^{241}Pu^a$	$^{235}U^a$	$^{240}Pu^a$	$^{238}U^a$	$^{239}Pu^a$
MSBR	^{233}U	^{235}U	$^{232}Th^a$	$^{238}U^a$	^{239}Pu

[a]Yield is from fission-spectrum-energy neutrons.

F7.6.4 PRINTED OUTPUT

A large quantity of printed output is available from ORIGEN-S. A total of more than 160 different types of tables presently may be printed, with possible options to print about 150 tables in a single subcase. Also, there are error or warning messages that may be printed. In general, the user may control the suppression or printing of each table, with a few exceptions. The tables (later referred to by group numbers) are divided into the following groups:

1. Concentration results during decay or non-irradiation, given either by quantity or converted to other units (in seven types of units).

2. Concentration results during reactor irradiation, by quantity (in one to three types of units as specified by requested options).

3. The k_∞, relative total neutron production and absorption results, and fractional neutron absorption by nuclide results.

4. Edits of the six library segments of the "card image" nuclear data library or the cross-section data of one or more burnup intervals of the binary library.

5. Photon rate and gamma-energy rate spectra for each library, in fixed energy group structure, tables for neutron production from spontaneous fission and (α,n) reactions, and neutron production rate spectra of the actinides. The 12 tables in this group may be obtained during the decay period only. They are suppressed or printed as a group. The reference to "photon and neutron table results" or "photon tables" in the input description means all tables of this group.

6. Photon rate and gamma-energy rate spectra of the sum of the nuclides from all three libraries or the spectra of the sum of the nuclides from a single library, at requested time intervals. The user may supply an energy group structure or, in some options, use the default. Three gamma line data bases are available: (1) The ORIGEN-S Photon Library (see Sect. M6.3); (2) ENDF/B file data for fission products only (see Sect. M6.6); and (3) the ORNL Master Photon Data Base (also see Sect. M6.7), which partly uses ENDF/B data, but principally applies data from the Evaluated Nuclear Structure Data File (ENSDF) at ORNL (supplemented with other photon data such as bremsstrahlung). The spectra in this group are termed "special gamma source spectra" in the input description.

7. Edits of photon data for each nuclide while producing new photon libraries (e.g., for an updated ORIGEN-S Library produced from the ORNL Master Photon Data Base or the ENDF data base).

8. Other variations to the spectra of Group 6. One option produces spectra in which only the nuclides having line data are included. Delayed decay spectra of the actinides may be obtained when special libraries have been made.

9. Integration over the time-step intervals, for decay period only, of the fission product nuclides and spectra. These "time integration" results may apply to all decay period fission product tables, which are included in the groups described above. This option simply adds "integral" table results to the output after all of the regular "instantaneous" results are printed for the first five groups. The spectra of Group 6 are only "integral" results. Except for MeV/fission units of Group 6, the units printed for "integral results" should be multiplied by seconds.

The results or edits in the above groups are separated into tables pertaining to each of the three libraries, except where specified otherwise. The majority of the tables may be suppressed or printed individually. Results in the first three groups are usually given for all elapsed times requested in the input (see 60** array in Data Block 6).

Note that there is a print limitation. Output results for Groups 1, 2, 3, 5, and 9 are subject to a fixed format, which does not permit the number of time steps printed to exceed ten for each subcase. The user may apply more than ten time steps when print is not requested or by simply using more subcases.

F7.6.5 CLARIFYING CONCENTRATION UNITS TO USE AND FLUX VS POWER

The ORIGEN-S code has been developed to solve a wide variety of isotope decay and build-up problems, including fuel and waste management, blending reactor streams, recycling actinides or molten salt, spent fuel gamma and neutron sources, fuel afterheat generation rates, source energies per fission, and thermocouple transmutations—to mention a few. Sometimes, the input involves a given neutron flux, and other problems require a power per basic unit of fuel. The units of nuclide concentrations input and output also should reflect the intent of the problem.

The mathematical model in the code compels the code to use atom-type units, such as gram-atoms or moles. The code also uses flux, converting input power to flux. If flux is input, the conversion is not needed. If power is input, it must equal the power in the total fuel concentration input. Then, normally the concentrations are input as grams or gram-atoms, instead of parts per million. When grams or gram-atoms are input, either grams or gram-atoms are permitted in irradiation period output tables while grams, gram-atoms, curies, and several other units are allowed in the decay period output. When atom ppm or weight ppm are the input units (i.e., for thermocouples), either of these units or atoms/(barn-cm) are the only units given in all of the output tables. It may lead to confusion to attempt to input both power and ppm units. When using the code for fuel management or spent fuel sources, the "unit of fuel" or "basis" can be printed out in a subtitle. This should pertain to the total fuel concentration input (i.e., total grams or gram-atoms). Reasonable quantities for the "basis" are metric ton heavy metal, kg fuel, fuel per assembly, quantity per fuel pin, or quantities per barn-cm. In cases for obtaining source energies per fission, the proper choice of concentration, σ_f, flux, and time should make the basis "the quantity producing one fission."

F7.6.6 CASES AND SUBCASES

The input data for a job may contain stacked "cases" and "subcases" as described here.

A "case" is defined as that part of a job that includes all of the problems solved after starting with both a different nuclear library and new material concentrations, unless the "blending feature" is used. The flag, NGO, is used to specify the type of the next problem. If NGO = 0, the following problem uses both new concentrations and a different library. If NGO = 0 and NOBLND = 1 (the flag set for "no blending"), the next problem is the start of a new case.

If a "blending case" is requested (specified by NOBLND > 1), even a problem starting with both new concentrations and a different library can be a subcase of the blended case. A new case starts after NGO = 0 only if the number of subcases where KBLEND was set positive equals the value of NOBLND.

F7.6.7 NUCLIDE OR ISOTOPE IDENTIFICATION NUMBER

A six-digit "nuclide" integer is used to identify each isotope including its isomeric state. This is called a "Nuclide ID No." in the input description. There is also an "Element ID No." The following equations are used:

$$\text{Nuclide ID No.} = IZ * 10000 + IW * 10 + IS$$

$$\text{Element ID No.} = IZ * 10000$$

where

- IZ = the atomic number, Z,
- IW = the mass number, A,
- IS = 0, for ground state,
- IS = 1, for metastable state,
- IS > 1, for additional metastable state levels.

F7.6.8 FORMAT OF INPUT DATA

Either the fixed-field, free-field, or user-field type of FIDO input system should be used, except for title cards or supplemental libraries. The FIDO input system is explained in Sect. M10.

Note that each parameter (or entry) is named and defined below in the order in which it appears in the data array. For applying fixed-field formats, data entries should be placed in successive data fields. If using free-field form, $$ or ** should be used with the array identifier, and at least one space should be skipped between data entries. Each data block contains one or more arrays followed by the data block terminator letter "T." Only the first 72 columns are allowed. Note that the word "card" is occasionally used. It should be interpreted to mean "card images" (or, the line typed on a terminal before the next carriage return).

The normal method of invoking ORIGEN-S is through the SCALE system. The SCALE driver requires a control card preceding the card input data and an "END" card as the last ORIGEN-S data card (with data for other codes following it, if desired). The complete ORIGEN-S cards are (the "=" may be replaced with "#")

=ORIGENS
(ORIGEN-S FIDO-type data)
END

The first and last cards begin in column 1. **Be sure to include** the "END" card. If it is omitted, the output contains only a list of the data.

F7.6.9 CONDENSED ORIGEN-S INPUT DESCRIPTION

Note: Default values are given in parentheses. (Assume that the data are required unless a condition is specified.) Also, while only a single * or $ is shown with each array identifier, be careful to use the **doubles**, ** and $$, if the **free-field** form of input is **intended.**

DATA BLOCK 1 – New Case. **Always** required in first case. If all defaults apply, enter \fBT\fR.

–1$ Maximum array storage size. (1 entry)

LNREAD Size of array storage requested, in words. (150,000)

0$ Data set unit numbers used in case, sometimes required. Where units are not used, or the defaults apply, unit numbers should **not** be entered. Most variables are referred to in later input data. (12 entries)

1. KOUT 5th entry in 3$ array. (6)
2. NDUM For supplementary FIDO edits. (13)
3. NPUN 16th entry in 56$ array. (0)
4. NDSETB 1st entry in 3$ array, if binary library. (21)
5. NDSETF 1st entry in 3$ array, if formatted library. (0)
6. NVERTR 32nd entry in 3$ array, if NVERT is positive. (0)
7. NVERTW 32nd entry in 3$ array, if NVERT is negative. (0)
8. NDFB 3rd entry in 81$ array, if binary library. (0)
9. NDFF 3rd entry in 81$ array, if formatted library. (0)
10. LDSET 2nd entry in 81$ array. (0)
11. NXTR Binary photon library unit no., required if LNGAM = 6, 11, 12, 13, 14, or 15, (1st entry in 81$ array). May use for read/write of concentrations. See "Detailed Input." (0)
12. NDISK Scratch (binary) data set unit number always required. (11)

1$ New case or blend option trigger. (1 entry)

NOBLND 0/1/N – job terminates/no blending/N streams blended. (1)

T Block terminator. This item is **always** required.

DATA BLOCK 2 – New Library. **Always** required in first case.

TITLEL — Title printed in library edit. Format (20A4)

2* — Required if NOBLND > 1. (NOBLND entries)

FACT — Fraction of each blended stream.

3$ — Library Constants. See Sect. M6 (e.g., for library sizes). (33 entries)

1. NDSET — Library unit number. Six unit numbers in 10$ array, if NDSET = -20. (28 if NTYPE=0; 30 if NTYPE>0)
2. NOLIB — Number of reactor libraries in NDSET. (4)
3. NTYPE — 0/>0 card image library/data position in binary library. (0)
4. NGRP — -N/0/N neutron spectra group structure from unit N/not used/from 84*. (-82)
5. KOUT — Printed output unit number. (6)
6. MPCTAB — 0/1 air, water hazards requested/not requested. (0)
7. INPT — 0/1 read photon library from NDSET/cards. (0)
8. IR — -1/0/1 print transition matrix and check branching fractions/do not print/print transition matrix. (0)
9. LPU — 0/N read all actinide data from NDSET/N actinides from user input. (0)

10-15. NN1,NN2,NN3,NN4,NN5,NN6:
NNI 1/0 print Ith library table/do not print. (0)

16. NN7 — Trigger for concentration units in 74* array (0):
0/1/2/3/4 units in gram-atoms/wt ppm/grams/atom ppm/curies.
17. NN8 — -1/0, suppress/print of library prologue. (-1)
18. ITMAX — Total number of library nuclides. (1706)
19. ILMAX — Number of library 1 nuclides. (692)
20. IAMAX — Number of library 2 nuclides. (132)
21. IFMAX — Number of library 3 nuclides. (882)
22. IZMAX — Number of off-diagonal nonzero matrix elements. (7500)
23. NREACT — Maximum number of reactions for any nuclide. (7)
24. NFISO — Number of fissile isotopes producing fission products. (5)
25. NELEM — Maximum atomic number in calculation. (99)
26. NMO — Month in date of library.
27. NDAY — Day in date.
28. NYR — Year in date.
29. NENAC — Number of actinide photon energy groups. (18)
30. NENLE — Number of light-element photon groups. (12)
31. NENFP — Number of fission product photon groups. (12)
32. NVERT — Integral Option Trigger:
-N/0/N request integral option (writing unit N)/not wanted/request integral option (reading unit N). (0)
33. NG — -N/0/N photon spectra group structure from unit N/not used/from 83*, required if LNGAM ≠ 0 or 15 (1st entry in 81$ array). (0)

Note: Skip option for entries 19, 20, 21, 29, 30, and 31: -1, skips library or photon part of library.

4* Library Constants, required if NTYPE = 0. (4 entries)

1. THERM — Ratio of thermal neutron cross section of 1/v absorber to 2200-m/s cross section. (1.0)
2. RES — Resonance flux per unit lethargy/thermal flux. (1.0)
3. FAST — 1.45 times ratio of flux > 1 MeV/thermal flux. (1.0)
4. ERR — Truncation limit. (10^{-25})

5$ Library Position Number, required if NTYPE = 0. (1 entry)

NLIBE — Reactor library position in NDSET (2):
1/2/3/4 for HTGR/LWR/LMFBR/MSBR

10$ Separate library unit numbers, if NDSET = −20. (6 entries)

54$ Special Options – not required. (12 entries)
May include 54$ in Data Block 5 if not using JOPT(1) or JOPT(9).

JOPT — Triggers to obtain special option.

JOPT(I) — N/0 request option/not requested. Entry positions (I) trigger the following: (1) compute k_∞, etc., (2) save concentrations, (3) save total gamma sources of libraries 1 and 3, (4) save (α,n) and spontaneous fission sources, (5) save combined gamma source, (6) save totals of nuclide tables N of each library, (7) save for element tables N, (8) CUTOFF as "% of the total" in place of units in Table F7.6.2, (9) use single fissile nuclide for computing γ-spectra/fission, (10) use single fissile nuclide for adjoint version of code, (11) use (α,n) reactions (for neutron spectra) from borosilicate glass in place of UO_2 medium, and (12) use 200-MeV/fission in place of computed energy per fission.

T — Block terminator. This is **always** required.

DATA BLOCK 3 – Actinide nuclide cards required only if LPU > 0.

6$ (LPU entries)

NEWCX — Nuclide ID numbers of actinides read in by cards.
T — Block terminator. This is required only if LPU > 0.

Extra Card Input: If LPU > 0, read LPU cards for cross-section data of the NEWCX nuclides.

DATA BLOCK 4 – Photon Energy Group Structures. **Always** required in first case.

First data array is always required. See "Detailed Input" (Sect. F7.6.10) to use other arrays.

35$ Required (1 entry):
0, if photon energy group structure and ^{235}U fission photon distribution is available for input library or input in 83* array;
1, if any group structures read in this data block. (0)

T Block terminator. This is always required.

Extra Card Input: If INPT = 1, read in entire photon libraries. (Fixed format)

DATA BLOCK 5 – New subcase with same library. **Always** required.

56$ Subcase Integer Control Constants. (20 entries)

1. MMN Number of irradiation intervals. (0)
2. MOUT Number of time intervals in subcase (10):
   0, and MSUB = 0, job terminator;
   0, MSUB > 0, writes results of step MSUB and unit NXTR.
3. INDEX 0/1 power read in 58*/read flux in 59*. (0)
4. NTABLE 0, any group 1 output printed, if not suppressed in 65$;
   1, print summary tables, per 65$. (0)
5. MSTAR Time period for CUTOFF, photon sources (1):
   0, cut-off feature not used, and JTO = 1 or 4.
6. NGO Next problem indicator (1):
   -1, new concentrations and same library;
   0, new concentrations and library;
   1, old concentrations and same library;
   2, same as NGO = 1, but old subcase flux, power, and accumulated burnup are zeroed;
   3, old concentrations and new library.
7. MPROS 0, for no continuous chemical processing;
   N, for N groups of elements in a processed group. (0)
8. NPROS 0 if MPROS = 0;
   N, the maximum number of elements in a process group. (0)
9. MFEED 0, for no continuous feed. (0)
   N, if N nuclides are continuously fed into system. (0)
10. MSUB 0, for new concentrations (last NGO = -1 or 0);
    N, if old concentrations are from time interval N;
    -N, where N means the same, but with batch processing;
    N, and MOUT = 0, writes results of step N on unit NXTR;
    N, and MOUT = -M, requests steps N to M, inclusive. (0)
11. NTERM Minimum number of exponential expansion terms. (21)
12. NSHRT Maximum number of short-lived precursors in chain. (100)
13. NXCMP Number of new nuclide or element concentrations. (0)
    Also, NXCMP can be used in restart option. See "Detailed Input."
14. NUNIT 1/2/3/4/5/6 time (in 60*) in s/min/h/d/y/other. (4)
15. NTI 0, no title cards read at Data Block 6;
    1, TITLE read;
    2, BASIS read;
    3, both read. (0)
16. NPUN 0/N no save/saves concentrations, etc., on unit N. (0)
17. JTO 0, all concentration (or Groups 1, 2 and 5) tables output;
    1, all output results suppressed except per 54$ and 82$;
    2, may suppress only by 65$ or 66$;

3, suppresses all except photon and neutron spectra tables;
4, suppresses photon and neutron tables and by 65$ or 66$. (2)

18. NUC — 0, suppresses "irradiation" nuclide tables;
1, suppressed only by 66$. (0)

19. NEL — Same as NUC for element tables. (0)

20. KBLEND — −1, if subcase uses total of previously blended streams;
0, no blended stream saved or used;
N, concentrations at time period, N, multiplied by next value of FACT and added as part of blend. (0)

57* Subcase Floating Point Constants. (5 entries)

1. TMO — Code uses TIME(1) − TMO as first interval in calculation. (0.0)
2. RHO — Total material density (g/cm^3). Needed for tables in units of atoms/barn-cm, if NN7 = 1 or 3. (0.0)
3. CUT — An option for deleting elements in tables under 66$ control. If the concentration in units of 74* is less than CUT for any element, print for the element is deleted. CUT is source fraction cutoff in decay subcase. (0.0)
4. FRACPW — (TIME(MMN) − TMO)/(sum of irradiation time of all irradiation subcases). (1.0)
5. TCONST — If NUNIT = 6, number of seconds in the special time unit.

T Block terminator. This item is always required.

DATA BLOCK 6 − Subcase Arrays and Titles. Required, if MOUT > 0.

TITLE Subcase Title, if NTI = 1 or 3. Format (20A4)
BASIS Basis of Calculation, if NTI = 2 or 3. Format (10A4)

58* Power required if INDEX = 0 and MMN > 0. (MMN entries)

POWER Thermal power in time intervals of 60*, in MW/BASIS (consecutive values or MMN*th* value cannot be zero).

59* Flux required if INDEX = 1 and MMN > 0. (MMN entries)

FLUX Thermal flux in neutrons/cm^2-s (consecutive values or MMNth value cannot be zero).

60* Printout Times. (MOUT entries)

TIME Elapsed times since beginning reference time. These are in a heading above table results. See TMO.

1*	Output Cutoffs – required if MSTAR > 0 and isotopes are requested in 65$. (7 entries)
CUTOFF	Cutoff values for deleting lines from 7 types of 65$ array tables. These are compared with results at time period MSTAR. CUTOFF may be either in the units of Table F7.6.2 or as "% of the total" for the table [see JOPT(8) in 54$ array].
62*	Removal Constants – required if MPROS > 0. (MPROS entries)
PRATE	Group removal constants in continuous chemical processing. See next two arrays.
63$	Number of Elements – required if MPROS > 0. (MPROS entries)
NOPROS	Number of Elements being processed in each group.
64$	Atomic Numbers – if MPROS > 0. (entries = MPROS*NPROS)
NZPROS	Atomic numbers of all processed elements in sets of entries equal to NPROS. After the corresponding NOPROS elements, remaining entries are "0."
65$	Decay Period Print Triggers – required if JTO = 2 or 4 and MOUT > MMN, for decay subcases. (63 entries)
NTO	Controls which decay period concentration (Group 1) tables are printed, if not suppressed as a group; 0, suppresses table denoted by entry position; 1, prints table denoted by entry position. (0)

If NN7 = 1 or 3 (3$, with input in ppm) use "Detailed Input" for limits on units.

Table F7.6.2 can be used to easily determine entry positions. Simply look under the desired library type listing for the entry giving the units wanted. New users should first read "Detailed Input" (Sect. F7.6.10).

66$	Irradiation Period Print Triggers – required if JTO = 2 or 4, MMN > 0, and NUC = 1 or NEL = 1 for irradiation subcases. (12 entries)
KW	Controls which irradiation concentration (Group 2) tables are printed, if not suppressed by MMN, JTO, NUC or NEL; 0, suppresses table denoted by entry position, 1, prints table denoted by entry position where units are g-atoms for positions 1, 5, or 9, 2, prints tables in grams for positions 1, 5, or 9. (0)

Table F7.6.2 Entry positions (65$) for print of decay tables in condensed input

	Light Element			Actinide			Fission Product		
	Nuc.	El.	Sum.	Nuc.	El.	Sum.	Nuc.	El.	Sum.
gram-atoms (moles)	1	2	3	22	23	24	43	44	45
grams	4	5	6	25	26	27	46	47	48
curies	7	8	9	28	29	30	49	50	51
$\alpha + \beta + \gamma$ watts	10	11	12	31	32	33	52	53	54
γ watts	13	14	15	34	35	36	55	56	57
m^3 air (dilute to RCG_a)	16	17	18	37	38	39	58	59	60
m^3 water (dilute to RCG_w)	19	20	21	40	41	42	61	62	63

Note that NUC = 0 will suppress all tables by nuclides and NEL = 0 will suppress those listed by elements. If NN7 = 0 or 2, only the entries giving gram-atoms or grams may be used; whereas, if NN7 = 1 or 3, only the other three are available.

Table F7.6.3 gives entry position. Look under the desired library for the entry giving the units wanted, in conjunction with setting NUC, NEL, NN7 and JTO properly.

Table F7.6.3 Entry positions (66$) for print of irradiation tables in condensed input

Units of Results	KW	Light Element	Actinide	Fission Product	NN7
g-atoms (moles)	1	1	5	9	0, 2, or 4
grams	2	1	5	9	0, 2, or 4
weight ppm	1	2	6	10	1 or 3
atom ppm	1	3	7	11	1 or 3
atoms/(barn-cm)	1	4	8	12	1 or 3

73$ ID of nuclides - required for new case or if NXCMP > 0 and last NGO = -1 or 0. (NXCMP entries)

INUC1 Nuclide ID number (if NEX1 = 1, 2, or 3) or element ID number (if NEX1 = 4) for the concentrations in 74*.

74* Concentrations required with 73$. (NXCMP entries)

XCOM1 Concentrations for nuclides and elements in 73$ in gram-atoms (NN7 = 0), wt ppm (NN7 = 1), grams (NN7 = 2), atom ppm (NN7 = 3), or curies (NN7 = 4).

**75$** Library kinds – required with 73$. (NXCMP entries)

NEX1 1/2/3 where nuclide ID number applies to Library 1/2/3 of Sect. F7.6.3.
4, for element in Light-Element Library.

76$ ID of nuclides – required if MFEED > 0. (MFEED entries)

INUC2 Same as INUC1, applied to continuous feed option.

77* Feed rates – required if MFEED > 0. (MFEED entries)

XCOM2 Continuous feed rates or increases in feed rates (gram-atoms/s per fuel unit).

78$ Library kind – required if MFEED > 0. (MFEED entries)

NEX2 Same convention as NEX1, applies to 76$

79* Element fractions – required if MSUB < 0. (NELEM entries)

FREPRO Fractions of elements retained in batch chemical processing, where the entry number is the element atomic number. (0.0)

81$ Gamma Source and Library Update Constants, required if NG ≠ 0 and LNGAM ≠ 0. (6 entries)

1. LNGAM 0/1/2/3/>3 no request/source from ENDF data/source from Master Photon Library data/source from ORIGEN-S data on NDSET/updates various libraries (see "Detailed Input"). (0)
2. LDSET Output gamma source unit number, if LNGAM = 1. (51)
3. NDF Input data base unit number, if LNGAM = 1 or 2. (26)
4. MNDF 2/1 – mode of NDF: card image/binary. (2)
5. N1MAX Maximum number of floating-point words for ENDF input, or set by code for other input data. (3000)
6. N2MAX Maximum number of nuclide photon lines in data. (1000)

82$ Time-Step Source Triggers – required if LNGAM = 1, 2, or 3. (MOUT entries) (0)

M(N) 0/1/2/4/5/6 – not wanted/request fission product source per fission/total source per second/light-element source/actinide source/fission product source, for N*th* time interval (if LNGAM = 1, 2, or 3).
M = 4, 5, 6 are not applied and, also, M = 2 denotes fission product source from ENDF data, if LNGAM=1. (Other options set by M are explained in "Detailed Input.")

83* Gamma Energy Group Structure, in eV and descending order.
(NG+1 entries, 3$ array) (required, if LNGAM ≠ 0, 3, or 15 and NG > 0).

84* Neutron Energy Group structure, in eV and descending order—required if NGRP > 0. (NGRP + 1 entries, 3$ array)

T	Block terminator. Required if block is input (MOUT > 0).
IA	One source title card for each 82$ request. A single library title card if LNGAM > 3. Format (20A4)
FORMG	Variable format of new library, if LNGAM = 4 or 5. Requires a blank card here if LNGAM = 6, 7, 8, 9, or 10. Format (18A4)
FORMT	Variable format – required if JOPT(2) > 0. Requires 3 cards. Format (20A4). The format used for concentrations saved in data set on unit NPUN as card images.

END OF CONDENSED INPUT INSTRUCTIONS

Be sure to add following SCALE control card:

END

F7.6.10 DETAILED ORIGEN-S INPUT DESCRIPTION

Either fixed-field, free-field, or user-field type of FIDO input system should be used, except for title cards or supplemental libraries. Note that each parameter (or entry) is named and defined below in the order in which it appears in the data array. In applying fixed-field formats, the user should place data entries in successive data fields. For the free-field form, $$ or ** should be used with the array identifier, and at least one space should be skipped between data entries. Each data block contains one or more arrays followed by the data block terminator letter "T" (or "iT," where i is the data block number).

Note: All available default values are in parentheses, following the data definitions.

Where a reference to a parameter in 56$ array is needed, the parameter's position is given in square brackets (for example, [10th] refers to tenth entry in 56$ array).

DATA BLOCK 1 – Start of First Case, **always.** If all defaults apply, enter **T.**

-1$	Maximum array storage size. (1 entry)
LNREAD	Size (in single precision words) of storage requested for all input data and arrays. The storage size actually reserved is the smaller of LNREAD and that available for the machine (or the machine control parameters). (150,000)
0$ Array	Case data set unit numbers, sometimes required. (Not required if reading **only** a standard ORIGEN-S library data set on NDSET, i.e., 21 through 28, and writing none.) The user may skip this array in the input (defaults apply) unless one of the following is used: the line gamma source option (81$ array), the integral option (32nd in 3$ array), or saving of data on NPUN. (12 entries)
1. KOUT	KOUT, 5th entry in 3$ array. (6)

2. NDUM — Unit number used to print FIDO edits starting with that of 35$ array. (13)
3. NPUN — NPUN, 16th entry in 56$ array, usually, for saving data on unit NPUN. (0)
4. NDSETB — NDSET, 1st entry in 3$ array. Not required when using SCALE procedure or script. (21)
5. NDSETF — Same as NDSETB except that it applies to card image data set. (0)
6. NVERTR — NVERT, 32nd entry in 3$ array, when NVERT > 0. (Meaning, NVERT has been written.) (0)
7. NVERTW — Same as NVERTR except NVERT < 0, when writing the integral library. (0)
8. NDFB — NDF, when LNGAM ≠ 0 and MNDF = 1, which are in 81$ array. (0)
9. NDFF — Same as NDFB except that MNDF = 2, for a card image gamma library. (0)
10. LDSET — LDSET, 2nd entry of 81$ array, and LNGAM ≠ 0. (0)
11. NXTR — Binary photon library or concentrations stored on this unit number, required if LNGAM = 6, 11, 12, 13, 14, or 15, or [10th] MSUB > 0 with [2nd] MOUT ≤ 0. In using restart option (i.e., NXCMP ≤ 0[13th]), the setting of NXTR negative is permitted but no longer required. Code will read unit number $|NXTR|$. (0)
12. NDISK — Unit number of a scratch data set needed in code. Not required to enter for SCALE procedure or script. (11)

1$ Array — Case control flag, always required. (1 entry)

ALL NEW CASES START HERE. (NGO = 0 and NOBLND = 1)

NOBLND — Blending and case control flag (1):
0, for normal termination of job;
1, for case with no blending;
N, if N streams are to be blended. (See KBLEND, 56$ array.)

T — Data block 1 terminator. This is always required.

DATA BLOCK 2 – Start of New Subcase Using New Nuclear Data (Reactor) Library. Start here only if last value of NGO = 0 or 3. (See NGO, 56$ array.)

TITLEL — Library Edit Title, always required. Read in the Format (20A4). Printed in library edit only.

2* Array — Required if NOBLND > 1. (NOBLND number of entries)

FACT — Fraction of each blended stream used in "blending cases," where the specified fraction is taken times all concentrations in the stream. These fractions are in the order pertaining to the subcases that have the flag KBLEND > 0, in 56$ array. (Omit if NOBLND = 1.)

3$ Array — Library Integer Constants, always required unless all defaults are proper. See override method below. If not the first subcase, the default values for all 3$ data except NGRP and the edit flags NN1 through NN6 are the values used in the last prior subcase. (33 entries)

1. NDSET — Library data set unit number. (See Sect. M6.)
–20, six separate card-image library data set unit numbers are entered into 10$ array. (28 if NTYPE=0, 30 if NTYPE>0)

2. NOLIB — Total number of reactor libraries in the data set, including those not used. Ignored if NTYPE ≥ 1. (4)

3. NTYPE — Trigger denoting library type or data position in library (0):
0, for card-image version (as described in Sect. M6);
N, if N>0, denotes binary library in which the cross-section data are in the Nth position (e.g., the Nth cycle) of a multi-burnup library;
N, if N<0 for future type of library obtained from code call to subroutine MORDAT.

4. NGRP — Applies to energy-group structure of neutron spectra. Required if [17th] JTO = 2 or 3. (-82)
–N, if the energy-group structure is taken from the SCALE Master Library on unit no. N;
0, if neutron spectra not wanted;
N, if the energy-group structure for N groups is input in 84* array.

5. KOUT — Unit number of ORIGEN-S output results, which may differ from that of FIDO output. (FIDO uses unit given by 1st entry of 0$ array before libraries are written, and unit NDUM, 2nd entry in 0$, thereafter.) (6)

6. MPCTAB — Option flag for calculation of inhalation and water ingestion hazards (0):
0, if these results are requested for a subcase using the library;
1, if calculation not requested. (Also, see 65$ data for each subcase. Storage saved, if suppressed here. However, code always executes properly for the "0" default.)

7. INPT — Library photon data input option (0):
0, if photon library read from NDSET;
1, photon libraries (files 4, 5, and 6) are read from cards following Data Block 4.

8. IR — Debug output option (0):
–1, invalid sum of decay branching fractions and transition matrix elements derived from libraries are printed;
1, transition matrix elements derived from the libraries are printed;
0, print is suppressed.

9. LPU — Actinide library data cross-section input option (0):
0, if entire actinide data from NDSET;
N, if cross sections from cards override library data for N actinide nuclides. The nuclide ID numbers are entered in 6$ array, and the new cross-section cards follow Data Block 3.

10. NN1 — Output option for the Light Elements and Structural Materials Nuclear Data Library (0):
1, table is printed;
0, print is suppressed.

11. NN2 — 1, Actinide Nuclear Data Library is printed;
0, print is suppressed. (0)

12. NN3 — 1, Fission Products Nuclear Data Library is printed;
0, print is suppressed. (0)

13. NN4 — 1, Light-Element Photon Library is printed;
0, print is supressed. (0)

14. NN5 — 1, Actinide Photon Library is printed, including neutron yield data, etc., if [2nd] MOUT > 0;
0, print is suppressed. (0)

15. NN6 — 1, Fission Products Photon Library is printed;
0, print is suppressed. (0)

16. NN7 — Indicator of type of units to be used for the concentrations in 74* array (for all subcases). (0)
0, input units are gram-atoms;
1, input units are weight ppm;
2, input units are grams;
3, input units are atom ppm;
4, input units are curies.

17. NN8 — Library output option (−1) the library history prologue and radioactive hazard library table are suppressed;
0, these are printed.

18. ITMAX — ≥ total number of NDSET library nuclides. This is sum of nuclides in the three libraries referred to below (ILMAX, IAMAX, IFMAX), exclusive of additions using LPU option. Library sizes are given in Sect. M6.2 (p. M6.2.1).
If NTYPE = 1, for binary library, many of these entries are not used. **See NOTE, at end of 3$ Array.** Also, the defaults in entries 18 through 31, inclusive, are satisfactory for card image libraries. (1706)

19. ILMAX — Same meaning as ITMAX applied to Light-Element Library;
−1, if the library is not wanted. (692)

20. IAMAX — Same meaning as ITMAX applied to Actinide Library;
−1, if the library is not wanted. (132)

21. IFMAX Same meaning as ITMAX applied to Fission Product Library;
-1, if the library is not wanted. (882)
(If none of the nuclides of a library are required for a case, both region size and computer time are saved by the corresponding setting of ILMAX, IAMAX, or IFMAX to -1.)

22. IZMAX Total number of reactions from one nuclide to another nuclide for all libraries. Code determines this value, as variable NON, for storage of permanent arrays so that it is satisfactory to input a somewhat excessive value. Code prints message if NON exceeds IZMAX, and states nuclide ID number. **Note:** The code adds 4*LPU to the input or default value. When in doubt, set IZMAX = 5*ITMAX for most libraries. (7500)

23. NREACT Maximum number of reactions (transitions due to neutron capture or decay) that any single nuclide in library will make. If too small, code increments NREACT by one and processes library again (five times before terminating). Do not set at less than 5 for usual libraries. Normally, the default is best. (7)

24. NFISO Number of fissionable isotopes in the reactor library for which fission product yields are given. These isotopes are built into the 25$ array for card image libraries. (5)

25. NELEM Largest atomic number of nuclides in all libraries. Maximum allowable value of NELEM is 99. (It is suggested that user not truncate libraries with NELEM, except in unusual cases in which the user is certain that the library retains all valid chains. The storage saved is normally not very important. (99)

26. NMO Month, for date nuclear data library was made. (0)

27. NDAY Day of month of library. (0)

28. NYR Year library was made. Date printed only if NN8 = 0. (0)

29. NENAC Number of energy groups in Actinide Photon Library. (18)

30. NENLE Number of groups in Light-Element Photon Library. (12)

31. NENFP Number of groups in Fission Products Photon Library. (12)
(If a photon library is not needed and the corresponding value of ILMAX, IAMAX or IFMAX was not set to -1, the photon part of the library can be skipped by setting NENLE, NENAC and/or NENFP to -1.)

32. NVERT Integral Option Trigger. (If used, requires entry for NVERTR or NVERTW in 0$ array). (0)
0, integral option not wanted;

±N, in addition to computing the regular "instantaneous" concentrations, the code computes results integrated over the interval of each time step using the Volterra multiplicative method, as applied by Lee[8] (for only the fission products during decay). The instantaneous concentration tables (for all units specified in 65$ array) are printed first, and following a message that integrals will be presented, the same type of fission product tables are printed with the integral results. Note that the units of these integral tables should be interpreted as the units shown times seconds.

-N, writes the utility submatrices data set on N. (Requires NVERTW, 7th in 0$ array.)

N, applies data set from N, using less CPU time. (Requires NVERTR, 6th in 0$ array. Never enter both NVERTW and NVERTR.)

The integral option is not operable with a fission product library that includes data for any transition that pertains to a change in mass number (A) [e.g., the library containing branching due to delayed neutron decay (described in Sect. M6.7)].

33. NG — Applies to energy-group structure of photon spectra, required if LNGAM ≠ 0 or 15 (1st entry of 81$ array). (0)

-N, if the energy-group structure is taken from the SCALE master library on unit number N;

0, if LNGAM = 0 or 15;

N, if group structure is input in 83* array.

Note on override of 3$ array by binary library data: This note applies to parameters ITMAX to NENFP (entries 18–31), inclusive. If NTYPE ≥ 1, the correct values of these parameters are supplied from the binary library data set and the user may **not** override these parameters with one exception: a −1 entry for NENAC, NENLE, and/or NENFP will skip the use of the specified photon libraries. Also, if NTYPE = 0, the defaults for ITMAX to NENFP are satisfactory.

4* Array — Library Floating-Point Constants, required if NTYPE = 0. (4 entries).

1. THERM* — Ratio of the neutron cross section for a 1/v absorber with a population of neutrons having a Maxwell-Boltzmann distribution of energies, which is specified by an absolute temperature, T, to the cross section with 2200-m/s neutrons.[7] An equation for computing THERM is

$$\text{THERM} = \sqrt{\frac{\pi}{4}\frac{T_o}{T}}, \; T_o = 293.15\,\text{K}$$

*THERM, RES, and FAST have meaning only for thermal reactors. For the LMFBR, the cross sections on NDSET are already spectrum averaged, and THERM, RES, and FAST are equal to 1.0. (Set by Code for LMFBR - do not enter.)

Default is 1.0. (See Data Note B, Sect. F7.6.12, on THERM, RES, and FAST application and Sect. F7.2.6 for additional theory.

2. RES — Ratio of the resonance flux per unit lethargy to the thermal neutron flux. (1.0)
3. FAST — 1.45 times the ratio of flux above 1 MeV to the thermal neutron flux. (1.0)
4. ERR — A truncation error limit below which the values computed by the code will be considered to be zero. If a zero is entered, the code changes to default value. If not the first subcase, the default value is the value used in the last prior subcase. Possibly set to 10^{-35} if MeV/fission spectrum or the Integral Method (32nd of 3$ array) is requested. (10^{-25})

5$ Array Library Position Number, required if NTYPE = 0. (1 entry)

1. NLIBE — Integer for reactor library type for this problem (2):
   1, for HTGR Reactor;
   2, for LWR Reactor;
   3, for LMFBR Reactor;
   4, for MSBR Reactor;
   -2, obsolete.

10$ Array Six library unit numbers, if NDSET = -20. (6 entries)

Often this data array is not required, since the total library will be contained in six sequential files which all have the same unit number:

1. Light-Element Nuclear Data unit number.
2. Actinide Nuclear Data unit number.
3. Fission Product Nuclear Data unit number
4. Light-Element Photon Data unit number
5. Actinide Photon Data unit number
6. Fission Product Photon Data unit number.

54$ Array Special Options, not required. (12 entries)
(May also include this array in Data Block 5 except if using a card-image library and this is the first request of options 1 or 9).

JOPT(I) — ≠ 0, request option I, as defined below for position I.
= 0, option I not requested. (At start, 0 is the default.)

I. Definitions Pertaining to Ith Position of 54$ Array

1. The k-infinities and total actinide and non-actinide absorption computed and printed for all time steps (requires MMN > 0).
   >0, uses built-in values of (neutrons/fission). Applies to actinide library of standard size and order, i.e., as described in Sect. M6.2.3.
   <0, uses values input in 121*, 122*, and 123* arrays (requires NTYPE = 0). Enter 54$ array only in Data Block 2, if JOPT(1) < 0.

±1, prints absorption fractions for each nuclide in descending order (using value at time step MSTAR) for each of the three libraries.
±2, prints absorption fractions for L.E. Library only.
±3, prints absorption fractions for Act. Library only.
±4, prints absorption fractions for F.P. Library only.
±5, prints total actinide and non-actinide absorptions and k-infinities only.

2. Save starting concentrations of subcase. See FORMT near end of input.

3. Save final total gamma sources of the light elements and the fission products (from Group 5, photon tables), corresponding to the order of the energy group structures for the two-card-image libraries. FORMAT (5E16.4)

4. Save total alpha-neutron and spontaneous fission neutron sources for all time periods. FORMAT (5E16.4)

5. Save total Group 5 gamma source of nuclides from all three libraries combined, in the order of current card image actinide library group structure.[1]

6. N = 3 × (Integer). If entry "N + 0, 21 or 42" for printing a table (by summary) is 1 in 65$ array and NPUN > 0 (16th entry in 56$ array), the total values in the tables denoted by entries N, N+21, and N+42 are saved on NPUN for all time periods. FORMAT (5E16.4).

7. N = 8, 11, 17, or 20. Save option with the same meaning as JOPT(6) except that it applies to total values of element tables where the printed values for charge, discharge, and all time periods are saved. FORMAT (1X, 6(1P,E10.2))

8. An option controlling meaning of cutoffs in 61* array. (0)
= 0, CUTOFF is given in units of Table F7.6.4;
= 1, CUTOFF is given as "% of the total" for the table.

9. An option for reducing isotopes yielding fission products to a single isotope. Look up the position of the isotope for the reactor (5$) in Table F7.6.1 in Sect. F7.6.3, and enter that position (1 through 5) here. Option is useful for reducing core storage in MeV/fission spectra cases.

10. Performs adjoint calculation in the "Adjoint Version" of Code.[29]

11. An option for specifying the type of medium, which contains the α-emitters producing (α,n) reactions, for computing nuclide neutron production rates, (α,n) spectra,and total neutron spectra. (0)

= 0, applies data for UO_2 medium with a fixed light-element (natural oxygen) dependence;
= 1, applies data for a typical borosilicate glass spectral distribution with (α,n) source strength dependent upon the composition of both light elements (for neutron yields) and all elements (for stopping powers). See Data Note C, Sect. F7.6.13.

12. Model for removable heat/fission. (0)
= 0, applies explicit time-dependent energy/fission;[2]
= 1, applies 200 MeV/fission, as done by initial ORIGEN version.[1] Always required when FLUX input, 59* array, with no fissionable isotope input.

Note: These option values are treated as decision indicators in all subcases of the case. Any of the indicators may be turned off by reinserting the 54$ array in Data Block 5 for any subsequent subcase. Also, any new option except JOPT(1) may be requested or turned on in later subcases.

121* Array Required if JOPT(1) < 0 (user wants to supply the actinide υ values).

YTN Thermal group values of ν (neutrons/thermal fission). Each entry is applied to the nuclide at the corresponding position in the Actinide Library (101 entries, in present library).

122* Array Required if JOPT(1) < 0.

YRN Resonance ν (neutrons/resonance fission).

123* Array Required if JOPT(1) < 0.

YFN Fast ν (neutrons/fast fission). See group definitions in 4* array.

T Data Block 2 terminator. This is **always** required.

DATA BLOCK 3 – Omit if LPU = 0 in 3$ array.

6$ Array Required if LPU > 0. (LPU entries)

NEWCX Nuclide ID Nos. for actinide library isotopes to be read in from cards, which must be placed between Data Blocks 3 and 4.

T Data Block 3 terminator. Required if LPU > 0.

Extra Card Input:

If LPU > 0, there must be LPU data cards here to override cross-section data of actinide nuclides. The format is given in Sect. M6.2.3.

DATA BLOCK 4 – Photon Energy Group Structures and Flag. Required in first case.

Almost always, the user should set LFLAG = 0, skip the other data, and terminate this data block with a T. Data here do **not** pertain to the making or use of new photon libraries per 81$ array. After photon library was produced by **user-supplied** data, **then** this data block would be needed.

35$ Array Always required. (1 entry)

LFLAG — 0, if no more data read in this block and case use default values. These are correct for ORIGEN-S Photon Libraries (Sect. M6).
1, if more data read in this block. (See Sect. M6.3 for explanation of data used here.) (0)

Warning: Never read photon data here unless a corresponding library has been made. (0)

36* Array Optional. (NENAC + 1 entries)

EACTGP — Photon energy group structure boundaries for actinide nuclides (MeV, in ascending order). Used in printed table column of photon tables.

37* Array Optional. (NENLE + 1 entries)

EGROUP — Photon energy group structure for light-element nuclides (MeV, in ascending order). Used in printed table column.

38* Array Optional. (NENAC entries)

SFGAMA — Photons per fission for ^{235}U in the group structure given by EACTGP (no longer used).

39* Array Optional. (NENFP + 1 entries)

EFPGRP — Photon energy group structure for fission product nuclides (MeV, in ascending order). Used in printed table column.

Note that any new group structure given in this data block (for printing new group structures by average energy) must be exactly the same as the group structure used in making the photon library.

T — Data Block 4 terminator. This item is **always** required.

Extra Card Input:

If INPT = 1 (7th entry in 3$ array), the entire photon library (files 4, 5, and 6) are read here. Formats are specified in Sect. M6.2.3.

DATA BLOCK 5 – Subcase Control Data. **Always** required.

This is the first block when starting a new problem with old nuclear data library. (Start subcase here only if last value of NGO = –1, 1, or 2, in 56$ data.)

54$ Array May be included (see Data Block 2).

56$ Array Subcase Integer Control Constants, always required. (20 entries)

1. MMN — Number of time intervals during irradiation period (0);
0, for post-irradiation or decay-only subcase.

2. MOUT Total number of time intervals in this subcase (10);
   0, for job termination (subcase starting with 56$ array);
   0, and MSUB > 0, the concentrations at last time step MSUB are written on unit number NXTR (in 0$ array). This "dummy" subcase gives the method for saving results in a binary data set. Only 56$ is read, with NGO = 1 plus the "T." Next 56$ is for regular, or another dummy, subcase.
   -N, and MSUB ≥ 0, the results in g-atoms for steps MSUB through N, inclusive, are written on unit number NXTR.

3. INDEX Method input for irradiation case (0);
   0, fuel specific thermal power per BASIS input in POWER, 58* array;
   1, thermal flux input in FLUX, 59* array.

4. NTABLE
   0, all isotopes and all times will be given in decay output, unless suppressed with flag in 65$ array or (17th entry of 56$ array) JTO (0);

   1, only summaries of most important isotopes at alternative time periods are output.

5. MSTAR Output suppression and photon source indicator. Code omits printing isotopes where values are below a cutoff (61* array) for time period MSTAR, and principal photon sources are printed for time period MSTAR.

   0, cutoff feature not used and JTO = 1 or 4, which suppresses photon tables. (1)

6. NGO Flag to indicate the type of the next subcase and data block the user must start using for new data (1):

   -1, if next problem has new initial concentrations, or has blend of old concentrations, and has same nuclear data library. Next subcase begins with Data Block 5.

   0, if next problem has new initial concentrations and a new library. If NOBLND = 1, next case begins with Data Block 1, 1$ array. If "blending case" not finished, subcase begins with Data Block 2. Never repeat 0$ array data except after "END" and another "=ORIGENS" card.

   1, for a "continuation" problem in which concentrations found in present calculation and same library will be used. Next subcase will begin with Data Block 5.

   2, for same conditions as NGO = 1 (the "continuation" problem), except that flux, power, and accumulated burnup from prior subcases are set to zero for use in obtaining averages and accumulated burnup of next subcase. Note that otherwise the flux or power is weighted by FRACPW in 57* array. Used, possibly, in alternating between irradiation and decay subcases.

3, for a "continuation" problem in which concentrations found in present calculation and a new library will be used. Next subcase begins with Data Block 2.

7. MPROS A "continuous chemical processing" option (0):

   0, for no processing;

   N, where N groups of nuclides are continuously removed by chemical processing during reactor exposure period only, and each group includes those elements with the same removal constant. See 62*, 63$, and 64$ arrays.

8. NPROS Used with MPROS (0):

   0, for no continuous chemical processing;

   N, where N is the maximum number of elements in any of the groups with same removal constant. See 64$ array.

9. MFEED A "continuous feed" option (0):

   0, for no continuous feed;

   N, where N nuclides are continuously fed into system, as in a fluid fuel reactor. See 76$, 77*, and 78$ arrays.

10. MSUB

    0, if new initial concentrations used in this problem (0);

    N, for a "continuation" subcase where the initial concentrations are taken from the time period N of the last subcase;

    -N, where time period N provides concentrations. However, specified factors of given elements are removed through batch processing. See 79* array for specifying the factors, if NLIBE $\neq$ 1. Special built-in factors are used if NLIBE = 1.

    N, and MOUT = 0, writes results of step N on unit number NXTR. Use MOUT = -M to request results for steps MSUB through M, inclusive, with MSUB = 0 permitted to denote the initial concentrations to subcase. See [2nd] MOUT for details.

11. NTERM Minimum number of terms to be allowed in series expansion of matrix exponential, needed to assure convergence for long nuclide chains. May need to change from default value for special cases. (21)

12. NSHRT Maximum number of short-lived precursors to a long-lived isotope in any decay chain. Suggest default. (100)

13. NXCMP Number of nuclides or elements for which new concentrations are used as initial conditions to this problem.

    See 73$, 74*, and 75$ arrays. (0)

    Always required for first subcase or if last subcase had a value of NGO = −1 or 0. Also, NXCMP can be used to start with the concentrations made on data set NXTR in a previous job, where MOUT and MSUB (of 56$ array) are input to properly write the concentrations from one or more steps. Set NXCMP ≤ 0 in this subcase. Those from the first step saved are used in this subcase if NXCMP = 0. The set of concentrations written in the |NXCMP| position (or, the | NXCMP | time a set was saved) on NXTR are used, if NXCMP < 0. Then, omit 73$, 74*, and 75$ arrays.

14. NUNIT Trigger specifying units of the times read in 60* array (4):

    1, for time in seconds;

    2, for minutes;

    3, for hours;

    4, for days;

    5, for years;

    6, if other units requested. This requires (1) a card for TUNIT near beginning of Data Block 6, and (2) a value for TCONST (5th entry in 57* array).

15. NTI Code for specifying the number of title cards read in for this subcase. These are defined in Data Block 6. (0)

    1, requires 1 card, for "TITLE";

    2, requires 1 card, for "BASIS";

    3, requires 2 cards, for both "TITLE" and "BASIS."

16. NPUN Save option (0):

    0, for no save;

    N, code will save on unit N the initial concentration values, gamma sources, and neutron sources as specified in the special options entered in the 54$ array in Data Blocks 2 or 5. Photon libraries made by proper request with LNGAM, 81$ array, are produced on unit N.

17. JTO "Master Control Flag for Printed Results"; used in conjunction with 65$ and 66$ arrays for print of Groups 1, 2, and 5, in Sect. F7.6.4. (2):

    0, all output concentration table results and photon tables are printed except those suppressed by setting MPCTAB = 1 in 3$ array or NTABLE = 1;

    1, suppresses all Group 1, 2, and 5 output table results;

    2, suppresses individual tables as specified in 65$ and 66$ arrays, MPCTAB (6th entry in 3$ array), and NTABLE (4th entry in 56$ array);

    3, suppresses all except the photon and neutron table results;

    4, suppresses photon and neutron table results and only the individual tables as specified in 65$ and 66$ arrays, MPCTAB, and NTABLE.

18. NUC Output option indicator used with option flags in 66$ data for "irradiation period" tables (0):

    0, suppresses all nuclide output tables during irradiation period;

    1, no suppression unless with 66$ array.

19. NEL Output option indicator used with 66$ array (0):

    0, suppresses all element output tables during irradiation period;

    1, no suppression unless with 66$ array.

20. KBLEND Used only in "blending case" (always zero if NOBLND = 1 in 1$ data) (0):

    -1, if this is a subcase of a blending case, where the initial concentrations in this subcase are the total of blended streams from previous subcases;

    0, where this subcase is not involved in blending streams in any way. This may be true in subcases within a blending case or in other cases.

    N, (then, NOBLND > 1), the concentrations after time period N will be multiplied by the next factor in FACT (2* array) and added to the concentrations being stored for use in a subcase where KBLEND = -1.

57* Array Subcase Floating-Point Control Constants, always required. (5 entries)

1. TMO Time subtracted from first time period in 60* array to give first time interval in the calculation (units given by NUNIT - 14th entry in 56$ Array). (0.0)

2. RHO Total density of material in system (grams/cubic centimeters). Required only if output tables requested in units of atoms/(barn-cm). (See 66$ array) (0.0)

3. CUT An output element deletion option, if applied during irradiation period. Its units should be the same as those of input concentrations in 74* array. Then if the concentration of an element discharged (time period MMN) is less than CUT, the line is deleted from the element output tables. Also, this line deletion applies to all isotopes of the element in the nuclide output tables. See 61* array and MSTAR for a different cutoff feature. The default for this use of CUT is 0.0. This option is not available for output in units of ppm or atoms/(barn-cm) as given in 66$ array.

   If CUT is applied in a decay subcase (MMN = 0), only the nuclides having an energy-group intensity exceeding the product of CUT times the total group intensity of all fission products are included as "Principal Photon Source" nuclides. (See Printed Group 5 in Sect. F7.6.4.) The default of this application is 0.05.

4. FRACPW [TIME(MMN) - TMO]/(total irradiation time in reactor) for a problem using "continuation" irradiation subcases. These values affect the computed average flux or power, used in converting photon release rates to photons/Ws. FRACPW values of different subcases (or cycles) are the weighting factors that are multiplied times average powers in deriving the average power of fuel over its total reactor residence time from cycle average powers. Note that because the code excludes any time-step power (or flux) $< 10^{-6}$ of the cycle average power in computing the cycle averages, the user should similarly exclude the corresponding time intervals in the numerator and denominator of FRACPW.

   0.0, if not the above type of problem. (1.0)

5. TCONST Number of seconds in the special time units used when NUNIT = 6 (14th entry in 56$ array). If NUNIT ≠ 6, TCONST is not used.

T Data Block 5 terminator. This is **always** required.

DATA BLOCK 6 – Subcase Array Data and Titles. Required if MOUT > 0.

Where a reference to a parameter in 56$ array is needed, the parameter's position is given in a square bracket (for example, [10th] refers to tenth entry in 56$ array).

TITLE Subcase Title, required if [15th] NTI = 1 or 3. The title is printed at top of each table of printed results. If NTI = 0 or 2, the title from the last subcase is used, and this may not be first subcase. Read in the Format (20A4).

BASIS Title (40 characters) that is the unit of fuel on which the calculation is based. This title will be printed as the basis for the calculation (e.g., "Metric Ton of Fuel Charged to Reactor"). The BASIS card is required if NTI = 2 or 3. If NTI = 0 or 1, the similar card from the last subcase will be used, or blanks are used for the first subcase. Read in the format (10A4).

TUNIT Name of special time unit (≤ 3 character length), included only if NUNIT = 6 [14th]. Read in Format (A3).

58* Array Required if [3rd] INDEX = 0 and [1st] MMN > 0. (MMN entries)

POWER Specific thermal power of fuel in each time interval ending with times given in 60* array. Units are: MW/unit of fuel. There may not be two consecutive zero-power values entered, and last value may not be zero. Requires at least one fissionable isotope input in 73$ array.

59* Array Required if [3rd] INDEX = 1 and [1st] MMN > 0. (MMN entries)

FLUX Thermal-neutron flux in neutrons/cm^2-s. Last value or two consecutive values may not be zero. Requires JOPT(12) = 1 if no fissionable isotopes are input in 73$ array.

60* Array Always required. ([2nd] MOUT entries)

TIME Elapsed times since beginning reference time. These are the times printed in a heading above output results. In computing each set of concentration results, the code uses time intervals equal to the difference between consecutive times with the exception that the first time interval = TIME(1) – TMO, where TMO is given in 57* array. The special case of TIME(1) = TMO is permitted.

61* Array Required if [5th] MSTAR > 0 and either isotope or summary table flags in 65$ array are set to 1. (7 entries)

CUTOFF Cutoff values for the 7 types of nuclide or summary output tables described for 65$ data in corresponding units. If the result for any isotope at time period MSTAR is less than CUTOFF for that table, the isotope is deleted from the table. (0.0)

62* Array Required if MPROS > 0. ([7th] MPROS entries)

PRATE A first-order removal constant in "continuous chemical processing" for each group or fuel stream corresponding to the groups of elements specified in 63$ and 64$ arrays. Removal constants have an effect identical to decay constants. The Mth entry in PRATE applies to Mth stream. Units of seconds^{-1} are required.

63$ Array Required if MPROS > 0. (MPROS entries)

NOPROS Number of elements being processed in each stream. The *Mth* entry applies to the *Mth* stream. See 62* and 64$ arrays.

64$ Array Required if MPROS > 0. (entries = MPROS*NPROS)

NZPROS Atomic numbers of all elements being processed in the streams where "continuous chemical processing" is applied. There must be [8th] NPROS number of entries for each group or stream. The position of each group should correspond to the entry position of the applicable values in NOPROS and PRATE. Where the number in a group is less than NPROS, the

remaining entries of the group should be zeros before starting next group. See 62* and 63$ arrays.

65$ Array Decay Period Print Triggers, required if [17th] JTO = 2 or 4. (63 entries)

NTO An output suppression array for all (Group 1) "non-irradiation" tables except the photon tables or those already suppressed with [4th] NTABLE = 1 and MPCTAB = 1 (6th entry in 3$ array):

0, suppresses the table (or the two summary tables) denoted by the entry position (0 is default, unless JTO = 0);
1, prints the output for the entry position. (If NN7 = 1 or 3, where input is in parts per million, only the first three entries in the set for each library have any effect. Tables controlled by other entries are not printed. If NN7 = 1 or 3, further control of output during exposure and decay periods is specified in 66$ array.)

A total of 84 tables are controlled with the 63 entries here. Separate tables are printed for each of the three libraries. They may be listed according to nuclides or elements. The computed quantities may be given in seven different types of units for all time periods or alternate time periods. The following abbreviations are used in Table F7.6.4: Nuc., for nuclides (or isotopes); El., for elements; and Sum., for summary tables. The trigger at the Sum. entry position produces two condensed tables, listed by both nuclides and elements at alternative time steps. The meaning of the relative inhalation hazard unit, "m^3 air (dilute to RCG_a)," is "cubic meters of air to dilute the radioactivity of the isotope's concentration to RCG_a." A similar meaning pertains to the seventh unit, for ingestion hazard.

Table F7.6.4. Entry positions (65$) for print of decay tables

	Light Element			Actinide			Fission Product		
Units of Results	Nuc.	El.	Sum.	Nuc.	El.	Sum.	Nuc.	El.	Sum.
gram-atoms (or 66$ units[a])	1	2	3	22	23	24	43	44	45
grams	4	5	6	25	26	27	46	47	48
curies	7	8	9	28	29	30	49	50	51
$\alpha + \beta + \gamma$ watts	10	11	12	31	32	33	52	53	54
γ watts	13	14	15	34	35	36	55	56	57
m^3 air (dilute to RCG_a)	16	17	18	37	38	39	58	59	60
m^3 water (dilute to RCG_w)	19	20	21	40	41	42	61	62	63

[a]If NN7 = 1 or 3 (input in ppm), these entries produce tables in units triggered by 66$ array and then no other units are permitted.

Further general explanations are given in Sects. F7.6.3, F7.6.4, and F7.6.5; the 66$ array description; and the "Master Control Flag for Printed Result," JTO, definition [17th]. This array is not needed if JTO = 1 (to suppress all of these output tables) or JTO = 0 (to print all of them). However, if JTO = 0, the code also uses this NTO array but changes the default from 0 to 1 (requiring an entry of 0 for every table suppression). The information in Table F7.6.4 can be used to easily determine entry positions. Simply look under the desired library type listing for the entry giving the units wanted. For example, to print the actinides by elements in units of grams, enter a "1" in the 26th position of data array.

66$ Array Irradiation Period Print Triggers, required if [17th] JTO = 2 or 4, [1st] MMN > 0, and [18th] NUC = 1 or [19th] NEL = 1 for irradiation subcases. (12 entries)

KW Controls which irradiation concentration (Group 2) tables are printed, if not suppressed by MMN, JTO, NUC, or NEL;
0, suppresses table denoted by entry position;
1, prints table denoted by entry position, where units are gram-atoms for positions 1, 5, or 9;
2, prints tables in grams for positions 1, 5, or 9. (0)

Note that NUC = 0 will suppress all tables by nuclides and NEL = 0 will suppress those listed by elements. If NN7 = 0, 2, or 4, only the entries giving gram-atoms or grams may be used; whereas, if NN7 = 1 or 3, only the other three are permitted. Also, elements are deleted from the tables when the element concentration does not exceed the value of CUT in 57* array.

If input concentrations are in parts per million (NN7 = 1 or 3), the units triggered by the 66$ array are the only units used in either the decay or the irradiation period (triggered with the first three entries for library in 65$ array).

Table F7.6.5 gives entry positions. Look under the desired library for the entry giving the units wanted, in conjunction with setting NUC, NEL, NN7, and JTO properly.

Table F7.6.5. Entry position (66$) for print of irradiation tables

Units of Results	KW	Light Element	Actinide	Fission Product	NN7
gram-atoms (moles)	1	1	5	9	0, 2, or 4
grams	2	1	5	9	0, 2, or 4
weight ppm	1	2	6	10	1 or 3
atom ppm	1	3	7	11	1 or 3
atoms/(barn-cm)	1	4	8	12	1 or 3

73$ Array Required for new case, [13th] if NXCMP > 0 and [6th] NGO = −1 or 0 in last subcase. ([13th] NXCMP entries)

INUC1 Nuclide ID number for all isotopes with non-zero concentrations in the problem being solved.

Note one exception: If the corresponding entry of NEX1 = 4 in 75$ array, INUC1 = 10,000 times the atomic number of the element in light-element library (the element ID number) and the code computes isotopic concentrations from the "natural abundances" in library.

74* Array Required with 73$ array. (NXCMP entries)

XCOM1 The concentration for the nuclide or element at the corresponding entry in 73$ array. If NN7 = 0, units of XCOM1 are gram-atoms per unit of fuel used in 58* (if power is input). If NN7 = 1, units are weight parts per million (wt ppm). If NN7 = 2, units are grams. If NN7 = 3, units are atom ppm. If NN7 = 4, units are curies.

75$ Array Required with 73$ array. (NXCMP entries)

NEX1 1, if corresponding entry in 73$ array is in Light-Element Library;
2, for Actinide Library;
3, for Fission Product Library;
4, for element when using relative abundance in Light-Element Library.

76$ Array Required if [9th] MFEED > 0. (MFEED entries)

INUC2 Follows same convention as INUC1 in 73$ array, but applies to nuclide with a "continuous feed rate."

77* Array Required with 76$ array. (MFEED entries)

XCOM2 Continuous feed rate (or, change in feed rate) in gram-atoms per second per unit of fuel for nuclide at corresponding entry in 76$ array. Units are changed, as for XCOM1, if NN7 ≠ 0. A special rule is used if this option was also requested in the previous subcase; then the data in XCOM2 are added to the previous rates or if XCOM2 is zero or skipped rates are unchanged.

78$ Array Required with 76$ array. (MFEED entries)

NEX2 Follows same convention as NEX1 in 75$ array but applies to 76$ array.

79* Array Required if [10th] MSUB < 0. (NELEM entries)

FREPRO The fraction of the concentration of an element that is retained in the stream being used in problem after "batch chemical processing." Entry number 1 applies to hydrogen and entry number N applies to element of atomic number N. (Sixth entry is for carbon, and 92nd entry is for uranium.) If the element is not present, a number must still be entered, although it has no effect. A conservative rule is to enter "1.0" for an element if none of it is known to be removed. (0.0)

81$ Array Required if (33nd entry in 3$ array) NG ≠ 0 and if (1st entry in 81$ array) LNGAM ≠ 0.

Gamma Decay Source or Library Update Constants (6 entries) – required for computing either the "special gamma source spectra" listed in Group 6 of Sect. F7.6.4, or updated photon libraries. The spectra obtained in the "photon table results" (of Group 5) are in a fixed group structure, apply to each library separately, are computed only during a decay subcase, and may use a less accurate data base. However, the more specialized spectra obtained with the option here have the following attributes:

1. Any energy group structure may be applied.

2. The user may select nuclide photon spectra from one of three different data bases (Sect. M6).

3. The Master Photon Data Base[30] may be more frequently and easily updated.

4. The spectra, except for that from ENDF/B data base,[2] can be obtained either for the sum of nuclides in each library, separately, or for the sum of nuclides in all three libraries.

5. The decay spectra may be computed during either an irradiation or a decay subcase. The spectra during decay periods may be applied to spent fuel shielding problems, while the spectra during irradiation represents the part of the gamma energy in the reactor contributed by decaying nuclides. (Note that an irradiation period spectrum does not represent the total gamma rays released in the reactor, which should also include the instantaneous gamma rays associated with fission and gamma emission during neutron capture.)

Gamma decay sources are requested by setting LNGAM to 1, 2, or 3 in this data array, to select the desired data base. Other options should be set in the 82$ array. Also, the 83* array group structure (unless NG is negative or LNGAM = 3), NG in the 3$ array, and title cards are required. The production of updated libraries is requested with LNGAM > 3.

1. LNGAM Type of procedure and data base requested. (Note that some of the procedures require an entry for either NDFB or NDFF, 8th or 9th entry in 0$ array – never both.)

   0, none requested, or omit 81$, 82$, and 83* arrays.

   1, applies the ENDF/B (currently, ENDF/B-IV) data base[2] to fission products (see Sect. M6.6). This procedure produces the following:

   a. printed fission product decay spectra as specified by 82$ and 83* arrays;

   b. saved card images (if NPUN ≠ 0, [16th]) including title, energy group structure in "eV," the spectrum in MeV/"unit" and photons/"unit" (see 82$ array, for "unit" definition);

c. individual nuclide gamma decay source data set on LDSET.

2, applies Master Photon Data Base. This procedure produces

a. printed decay spectra per 82$ and 83* arrays;

b. saved card images, similar to LNGAM = 1 (if NPUN ≠ 0, [16th]).

3, applies ORIGEN-S photon-yield libraries that were previously produced (for current libraries in code package being issued or in a case in which LNGAM > 3). The data base is contained in the library denoted by NDSET, first entry of 3$ array. Note: The 83* array is not required. The procedure produces

a. printed decay spectra per 82$ array and fixed group structure of library;.

b. saved card images (if NPUN ≠ 0, [16th]).

4 through 14, inclusive (see differences below) invokes procedures for making new photon libraries for later use as either a card image or binary data set (specified later, by NDSET, 1st entry in 3$ array). A new library edit of nuclide data, as photons/disintegration by energy group, is always printed. All of these procedures require

a. NG ≠ 0, 33rd in 3$ array;

b. 83** array, group structure (may use default by omitting or input from unit number |NG|);

c. IA, the title card described below;

d. Any ORIGEN-S case setup using a library that includes the separate-type libraries of all nuclides wanted.

Additionally, if LNGAM = 4, 5, 6, 7, 8, 9, or 10, the following are required:

a. NPUN ≠ 0, [16th], except if LNGAM = 6.

b. FORMG, the variable format described below in the input following Block 6.

Or, if LNGAM = 6, 11, 12, 13, 14, or 15, a binary library is made on unit NXTR, 11th entry in 0$ array.

4, applying the ENDF/B data base, a card image library is made (on NPUN) for all fission product nuclides having either a non-zero spectrum or total gamma energy given on NDF. The format of the set of data for each nuclide is given by FORMG (input following Data Block 6) starting with the nuclide ID number as an integer and followed by the nuclide's spectrum in ascending energy order (as required for ORIGEN card image photon libraries). The library is printed, also.

5, applying the ENDF/B data base, a card image library is made (on NPUN) containing nuclides from the data base (on NDF) having gamma line spectra **only** (180, presently). Format FORMG is used, as with LNGAM = 4, with two changes. The first record contains NG plus the group structure from 83* array followed by the nuclide spectra records. Also, the nuclide spectra are in descending energy order. The library is printed.

6, applying the ENDF/B data base, a binary library is made on NXTR, 11th entry in 0$ array. It contains all nuclides, the same as with LNGAM = 4. The spectra are in descending energy order.

Although format FORMG is ignored, a dummy (blank) card is required.

Note concerning LNGAM procedures 4, 5, and 6: No bremsstrahlung X-rays are included. Since internal conversion energy of beta radiation has been excluded from the spectra data in the ENDF/B files, an approximation of the K- and L-shell x-rays are included. Where no line data are given, and LNGAM = 4 or 6, the total disintegration is placed in the energy group containing the total gamma energy or made a single line on LDSET.

7, applying the Master Photon Data Base, a card image library is made (on NPUN) for all three of the libraries. This option can be used to produce new ORIGEN-S Photon Libraries in the group structure specified by the 83* array (for $10 \leq NG \leq 12$). The libraries contain data for each nuclide that is contained both in the library denoted by NDSET (1st entry in 3$ array) and in the Master Photon Data Base on NDF (3rd entry in 81$ array). Nuclide data are omitted for nuclides with no spectrum available. This is unlike LNGAM = 4, in which a single group spectrum at the total gamma energy is used, when there is no spectrum for the nuclide. Thus, later cases using the photon libraries made here do not include energy from the omitted nuclides (which may be small) in the photon table results. However, special gamma source spectra that are invoked with LNGAM = 3 and positive values of M (82$ array) in the input for later cases will cause the spectra to be renormalized to include the energy from these omitted nuclides. Also, the total

energy of the omitted nuclides is printed. This method of normalization, compared with that from LNGAM = 4, was found to improve results, sometimes considerably, in applications to common shielding problems. (Also, the discerning user may note the differences, usually small, between Group 5 and 6 tables, which simply results from the improved normalization model.)

8, applying the Master Photon Data Base, a card image library ($1 \leq NG \leq 12$) is made for the Light-Element Library only. See LNGAM = 7 for further details. Options of LNGAM = 8, 9, and 10, in separate cases, are required, in place of LNGAM = 7, to make the libraries in the two different group structures of the initial version of ORIGEN.

9, applying the Master Photon Data Base, a card image library ($10 \leq NG \leq 18$) is made for the Actinide Library. See LNGAM = 7, for further details.

10, applying the Master Photon Data Base, a card image library ($1 \leq NG \leq 12$) is made for the Fission Product Library. See LNGAM = 7, for further details.

11, applying the Master Photon Data Base, an updated version of the photon spectra data in the input ORIGEN-S Binary Library is made (on NXTR) for **all three** libraries. The group structure is specified on unit $|NG|$ or by the 83* array. See LNGAM = 7, for further details. No limits are required for NG if LNGAM $\geq$ 11.

12, applying the Master Photon Data Base, a binary library is updated for the Light-Element Library only. Options 12, 13, and 14, in separate cases, may be used to apply different group structures. See LNGAM = 7 and 11 for further details.

13, applying the Master Photon Data Base, a binary library is updated for the Actinide Library only. See LNGAM = 7 and 11 for further details.

14, applying the Master Photon Data Base, a binary library is updated for the Fission Product Library. See LNGAM = 7 or 11 for further details.

15, the "card image" mode of the Master Photon Library (on NDF, 3rd in 81$ array) is converted to the binary mode (on NXTR, 11th in 0$ array). The "mode" of the input data base is denoted by the input MNDF, 4th in 81$ array. The application of the binary compared with the card image mode is more efficient, using less computer time and fewer I/O requests. An edit is printed (5,000 to 10,000

lines) by setting the unit number of the output photon library, NXTR = 40.

2. LDSET — Output nuclide line-gamma source unit number which applies for LNGAM = 1 only. (Requires entry for LDSET in 0$ array unless a DD DUMMY is used in IBM JCL for LDSET.) (51)

3. NDF — "Master Photon Data Base" or "ENDF/B Processed Data Base" input library unit number. (Requires entry of NDFB or NDFF in 0$ array – see MNDF.) (26)

4. MNDF — 2/1 – input data base library in card image/binary mode. If MNDF = 2, enter NDFF, 9th in 0$ array. If MNDF = 1, enter NDFB, 8th in 0$ array. (Never enter both.) (2)

5. N1MAX — Maximum number of floating-point words in the input "ENDF/B Processed" data base record, for LNGAM = 1, 4, 5, or 6. Otherwise, code sets the value of N1MAX to a proper size. (3000)

6. N2MAX — Maximum number of gamma lines for any nuclide in the data base. (1000) (The N1MAX/N2MAX defaults supply a proper storage space for current data base sizes.)

82$ Time-Step Source Trigger required if LNGAM = 1, 2, or 3. (MOUT entries) (0)

M(N) 1 through 6, invokes procedure specified by LNGAM, producing gamma decay source spectra for nuclide concentrations of the Nth time step (where N pertains to the Nth entry). All non-zero values of M should be equal. One IA title card is required for each non-zero entry. If LNGAM > 3, omit M unless M(1) is set to 21.

0, no source requested for the time step.

1, requires LNGAM = 1, 2, or 3, producing a special fission product spectrum for the time step. The units of printed spectra are MeV/fission and photons/fission. Do not use this option unless the ORIGEN-S case was set up to force the units to be correct (usually for one fissile isotope). See Data Note A (Sect. F7.6.11).

2, invokes the procedure requested by LNGAM = 1, 2, or 3, which produces a gamma source spectrum for the Nth time steps. The units of the printed spectra are MeV/s and photons/s. This source production option is more general than that resulting from M = 1, and the spectrum from any irradiation or decay time step may be requested. There is a difference, depending upon LNGAM, in the number of nuclides included in the source spectra; for LNGAM = 1, using the ENDF/B data base, the source pertains to the sum of all fission products only; and for LNGAM = 2 or 3, using either the Master Photon Data Base or the ORIGEN-S photon libraries, the source pertains to the sum of nuclides in all three libraries. Sources for separate libraries may be requested with other values of M. There are two different

treatments used to account for the gamma energy of nuclides which have no spectrum data included in the data base:

a. For LNGAM = 1, the spectrum is increased by one photon/disintegration in the group that includes the total gamma energy of the nuclide having no spectrum data.

b. For LNGAM = 2 or 3, the ratio is computed which equals the sum of the gamma energy of all nuclides divided by the sum of the gamma energy of only those nuclides having photon data. After the total spectrum of nuclides having data is computed, it is renormalized by multiplying by the above energy ratio. The energy is conserved, with the uncertain fraction of the spectrum having the same distribution as that produced from all nuclides that have spectrum data. The total energies are printed for the sum from all nuclides both with and without spectrum data.

Note of warning in using LNGAM = 3: This is a request for summing the spectra computed from the three separate ORIGEN-S libraries. The request **implies** that the user is aware that the group structures of the three ORIGEN-S photon libraries are compatible (either the same, or one is a subset of another and the maximum boundaries are equal). The group structures are compatible in the three current ORIGEN-S photon libraries in the code package being issued.

3, produces the gamma spectra of the decay of actinide neutron captures from data in a special library. This option is restricted to a very limited use and requires that the ENDF data file be processed. Similar results can now be computed from the Master Photon Data Base.

4, produces the gamma source for only the nuclides included in the Light-Element Library. It may be requested only for LNGAM = 2 or 3.

5, produces Actinide Library gamma source for LNGAM = 2 or 3.

6, produces Fission Product Library gamma source for LNGAM = 2 or 3.

(Important note: The user may not change to different non-zero values of M at later time steps.)

20 + M, or 21, triggers the printout lines stating that the Master Photon Data Base contains, for a given nuclide, gamma-ray intensity data at an energy outside the range of the requested group structure. The message begins with "Photon could not be binned." First, for LNGAM = 2, determine (from the above), the value of M desired and add 20. Set to 21 if LNGAM > 3. The option applies only to cases using the Master Photon Data Base, or LNGAM = 2 or LNGAM > 3. (Note there are pages of lines written if energy range does not start near zero; thus, when running several cases, the user may not find it desirable to use this trigger except for a single trial case.)

−1, is the same as M = 1 except that only the nuclides with gamma-line data are used in the LNGAM procedure.

-2, -4, -5, and -6, produce gamma-decay source spectra computed from only those nuclides that have spectrum data. This step allows the user to add in other data for those nuclides having no spectrum data.

83* Gamma Energy Group Structure, in eV, for spectra or library updates requested if LNGAM ≠ 0, 3, or 15. Boundaries are in descending order. (NG + 1 entries, 33rd in 3$ array.) Required only if NG > 0.

The energy group structures which correspond to that of input ORIGEN-S photon libraries (on NDSET) are the defaults obtained by skipping this array, after the proper input of NG (33rd in 3$ array). NG = 12 obtains the Light Element and Fission Product structures, while NG = 18 obtains that for the actinides.

84* Neutron Energy Group Structure, in eV, for neutron spectra requested by JTO = 2 or 3, and NGRP > 0. Boundaries are in descending order. (NGRP + 1 entries, 4th in 3$ array.) Required only if NGRP > 0.

T Data Block 6 terminator, required if block input (MOUT > 0).

IA Title cards for each time period that a gamma source spectrum is requested, in order of the periods, or library title card. The number of cards must be equal to the number of non-zero entries in 82$ array and have only one card per title. Also, producing a library with LNGAM > 3 requires a single title card. It is added to the title cards of a binary ORIGEN-S library. Format (20A4)

FORMG A card that is either "blank" or contains a variable format used to write libraries produced by LNGAM = 4 through 10, inclusive. A blank card is required if LNGAM = 6. Also, when using options 7 through 10 for making ORIGEN-S photon libraries, simply use a **blank card** for FORMG. When making photon libraries for other purposes and when LNGAM = 4 or 5, the desired variable format is required. The format should fit a word list starting with the nuclide ID number (an integer), followed by the photons/disintegration for each of the NG groups. All data are in ascending energy order except for LNGAM = 4, in which they are in descending order. Note that data cards produced for uses by codes other than ORIGEN-S will have several "header" cards, required for ORIGEN-S, before the start of nuclide data. Format (18A4).

If JOPT(2) > 0 in 54$ array, three format cards for nuclides of the three libraries are required as follows:

FORMT Read in (18A4) format. These are three variable formats used for saving nuclide concentrations. The results are saved for all nuclides in the order of light elements, actinides, and fission products, with all nuclides in the library listed in one program statement (i.e., first nuclide ID number, its concentration in gram-atoms, next ID number, etc.). (3 cards required.)

This is the **End** of **Input** data of case/subcase. Be sure to add following SCALE control card:

END

F7.6.11 DATA NOTE A: NORMALIZING SPECTRA TO ONE FISSION

This data note mainly concerns the use of M(N) = 1 in the 82$ array. It was initially utilized to compute gamma source spectra produced per fission of a specific nuclide, resulting from the ENDF/B processed data base. The procedures explained here could similarly be applied to cases using other data bases, as specified by different input entries for M and LNGAM.

The most frequent application of this option is to compute total production of fission product photons, D_T, or gamma energy, E_T, during the decay intervals $T_i - T_{i-1}$, following a fissile isotope's exposure to very small and constant neutron flux, normalized to one fission. D_T and E_T apply to a single fission product, or the summation of all fission products. Let $\dot{D}$ and $\dot{E}$ be the time rate derivatives of D and E, respectively, and $\dot{D}$ be constant between T = 0 and T = T_{exp}; then

$$D_T = \frac{1}{N_f} \int_0^{T_{exp}} \int_{T_{i-1}+T}^{T_i+T} \dot{D}\, dt\, dT\ , \qquad \text{(F7.6.1)}$$

and

$$E_T = \frac{1}{N_f} \int_0^{T_{exp}} \int_{T_{i-1}+T}^{T_i+T} \dot{E}\, dt\, dT\ , \qquad \text{(F7.6.2)}$$

where N_f is the number of fissions during T_{exp}, the exposure time. If x_0 is the fissile isotope concentration (undepleted) in gram-atoms, σ_f is its fission cross section in barns, A_0 is the Avogadro number, ϕ is the flux, and T_{exp} is the exposure time in seconds, then:

$$N_f = x_0 A_0 \sigma_f (10^{-24}) \phi T_{exp}\ . \quad \text{(Code uses } A_0 = 6.023 \times 10^{23}\text{)} \qquad \text{(F7.6.3)}$$

There are two methods of setting up the ORIGEN-S case for computing D_T and E_T.

(a) Adjoint Input Method:

This method applies to short exposure pulses only. Choose x_0, σ_f, ϕ, and T_{exp} so that

$$\frac{N_f}{T_{exp}} = x_0 A_0 \sigma_f \phi (10^{-24}) = 1 \text{ fission/s, and } T_{exp} = T_i - T_{i-1}\ . \qquad \text{(F7.6.4)}$$

Follow the exposure case with a decay subcase, using the discharge concentrations, and set T(1) to $T_i - T_{i-1}$ s, and M(1) = 1. [T(1) = 10^{-12} s is all right when $T_i - T_{i-1} = 0$.] Then, printout of D_T and E_T at time step I can be normalized to photons/fission and MeV/fission. Avoid depletion by making $\sigma_f (10^{-24}) \phi\ T_{exp} \leq 10^{-6}$. For example, setting $\sigma_f = 1000$, $\phi = 1$, and $x_0 = 10^{21}/A_0 = 1.66044 \times 10^{-3}$ yields one fission/s. It is best to set ERR, the 4th entry in 4* array, to about 10^{-35}. The user should always use at least ten time steps in T_{exp} (and several steps for long T_{i-1}) and validate the case with another one in which the number of T_{exp} steps is increased by 50%, or at least ten. This method may save computer time compared with the "integral method" for long integral intervals. Also, it can be used for different decay times to obtain (MeV/s)/(fission/s). However, it lacks the reliability of the integral method and requires $T_{exp} = 0$.

(b) Integral Method:

By setting NVERT ≠ 0, 32nd of 3$ array, the "Integral Option" is invoked. Then, a single fission is required ($N_f = 1$) with T_{exp} set small (approximately 10^{-6} s) for a "pulse" problem or T_{exp} set to larger finite values. The values of T in the decay subcase that follows are the T_{i-1} and T_i limits in the above integrals. If M(I) = 1 and the case is set to force $N_f = 1$, the units of MeV/fission apply to the time-integrated spectrum between the limits T(I–1) and T(I). For example, if $T_{exp} = 10^{-6}$, $\sigma_f = 1000$, $\phi = 1$, and $x_0 = 10^{27}/A_0$, one fission is produced. Cases have been computed with T(I) – T(I–1) as large as 10^{15} s. It is best to set ERR, 4th entry in 4* array, to about 10^{-35}.

F7.6.12 DATA NOTE B: WEIGHT FACTORS: THERM, RES, AND FAST

Probably the most difficult to obtain input data for ORIGEN-S are the spectral parameters THERM, RES, and FAST, which are needed in calculations pertaining to HTGR, LWR, and MSBR reactors. (The LMFBR library contains fixed cross-section values, and they cannot be altered from the input of THERM, RES, and FAST.)

ORIGEN-S requires data for all significant nuclide transition rates, by isotopic decay or neutron absorption. Isotopic decay rates are constant. While neutron reaction rates may vary with time, the ORIGEN-S model requires that a constant, or effective, reaction rate be used during the period for which the library is applied. Ideally, the computed results approach the correct solution as an increased number of different libraries, providing more closely approximated reaction rates, are used with smaller time intervals. Furthermore, to compute a time-dependent effective cross section, $\sigma(t)_{eff}$, would require a time-dependent fine-group neutron flux spectrum and fine-group cross-section data. Then, $\sigma(t)_{eff}$ is given by

$$\sigma(t)_{eff} = \frac{\sum_i \phi(t)_i \sigma_i(t)}{\sum_i \phi(t)_i} . \qquad \text{(F7.6.5)}$$

Procedures which, in principle, follow this model have been developed by computing weighted cross sections for reactor cells with the NITAWL-II and XSDRNPM codes and incorporating them into ORIGEN-S libraries with the COUPLE code. The unification of the procedure has been developed into the SAS2 module of the SCALE system so that a single case produces a series of time-dependent libraries for ORIGEN-S.

The binary libraries produced by COUPLE have THERM, RES, and FAST "built in," in effect. Other special card image libraries, for which the values of THERM, RES, and FAST are included for specific types of reactors, have been produced.

Many users have only the original ORIGEN nuclear data library, normally distributed with the ORIGEN-S or ORIGEN codes. Calculations of 33,000 MWD/MTU PWR fuel burnup have frequently been made using this original library and the values THERM=0.632, RES=0.333, and FAST=2.00.

The following may be used when the neutron flux spectrum is available. First, the definitions of THERM and RES are discussed with respect to the definitions of the data in the original ORIGEN-S library. The one-group, or effective cross section, σ_{eff}, and thermal flux, ϕ_{th}, as used by ORIGEN-S relate to THERM and RES as follows:

$$\sigma_{eff}\,\phi_{th} = \text{THERM} \times \sigma_0 \times \phi_{th} + \text{RES} \times \text{I} \times \phi_{th} , \qquad \text{(F7.6.6)}$$

where

$$\sigma_0 = 2200 \text{ m/s cross section}$$

$$I = \int_{0.5\ eV}^{\infty} \frac{\sigma(E)}{E}\, dE$$

$$\phi_{th} = \int_0^{0.5\ eV} \phi(E)dE \ . \qquad \text{(F7.6.7)}$$

ORIGEN-S uses the convention of normalizing cross sections to thermal flux and requiring thermal flux or power to be input. The library contains only the two-group values σ_0 and I for data applied to neutron absorption reactions such as (n,γ) or (n,f). This convention permits the direct application of values per σ_0 and I from student references such as BNL-325. Reaction rates, R, which are computed by Eq. (F7.6.6) in ORIGEN-S, are theoretically defined by

$$R = \int_0^{\infty} \phi(E)\sigma(E)dE = \int_0^{0.5\ eV} \phi(E)\sigma(E)dE + \int_{0.5\ eV}^{\infty} \phi(E)\sigma(E)dE \ . \qquad \text{(F7.6.8)}$$

THERM and RES—which actually vary with isotope, reaction type, concentrations and geometry—are simplified by the following assumptions. It is assumed that thermal reaction rates follow that of a 1/v absorber, in defining THERM. Thus, if E_0 is the reference energy of σ_0

$$\sigma(E) = \frac{\text{constant}}{v} = \frac{C_1}{\sqrt{E}}$$

$$C_1 = \sigma_0 \sqrt{E_0} \ , \qquad \text{(F7.6.9)}$$

$$\sigma(E) = \frac{\sigma_0\sqrt{E_0}}{\sqrt{E}} \ . \qquad \text{(F7.6.10)}$$

Equating the first terms of the right-hand side of Eqs. (F7.6.6) and (F7.6.8) and using Eq. (F7.6.10):

$$\text{THERM} \times \sigma_0 \times \phi_{th} = \sigma_0 \sqrt{E_0} \int_0^{0.5\ eV} \frac{\phi(E)}{\sqrt{E}}\, dE \ . \qquad \text{(F7.6.11)}$$

Rewriting this equation in a more useful form for the user having neutron flux group data, where groups 1 to n include the thermal groups (below 0.5 eV):

$$\text{THERM} = 0.15906 \sum_{i=1}^{n} \frac{\phi_i}{\sqrt{E_i}} \Big/ \sum_{i=1}^{n} \phi_i \ . \qquad \text{(F7.6.12)}$$

where E_i is derived by some logical method for representing the energy of each group.

Also, THERM can be obtained through the inclusion of a 1/v absorber material ($\sigma_0 \equiv 1$) in the neutron spectrum calculation. THERM corresponds to the spectrum-averaged cross section of such a material in the thermal energy range, or,

$$\text{THERM} = \sum_{i=1}^{n} \phi_i \, \sigma(1/v)_i \Big/ \sum_{i=1}^{n} \phi_i = \sigma(1/v)_{th} \, . \qquad \text{(F7.6.13)}$$

RES is derived by first equating similar terms of Eqs. (F7.6.6) and (F7.6.8):

$$\text{RES} \times I \times \phi_{th} = \int_{0.5 \text{ eV}}^{\infty} \phi(E) \, \sigma(E) \, dE \, . \qquad \text{(F7.6.14)}$$

The definition of I implies a 1/E weighted flux > 0.5 eV,

$$\phi(E) = \text{Constant}/E = C_2/E \, . \qquad \text{(F7.6.15)}$$

Substituting Eqs. (F7.6.15) and (F7.6.7) into (F7.6.14):

$$\text{RES} \times I \times \phi_{th} = C_2 \int_{0.5 \text{ eV}}^{\infty} \frac{\sigma(E)}{E} \, dE = C_2 \times I \, ,$$

or

$$\text{RES} = C_2/\phi_{th} \, . \qquad \text{(F7.6.16)}$$

Since C_2 is constant for all E in $\phi(E)$, C_2 is computed by integrating (F7.6.15) over any limits E_1 to E_2:

$$\int_{E_1}^{E_2} \phi(E) \, dE = C_2 \int_{E_1}^{E_2} \frac{dE}{E} = C_2 \, \ell n(E_2/E_1) \, ,$$

or

$$C_2 = \frac{\int_{E_1}^{E_2} \phi(E) dE}{\ell n(E_2/E_1)} \, . \qquad \text{(F7.6.17)}$$

This result is due to the 1/E weighting assumption. If C_2 were always constant, E_1 and E_2 could denote any epithermal energy range. In practice, with $E_1 = 0.5$ eV, C_2 was observed to vary about 10 to 15% in changing E_2 from 1 to 20 MeV. It appears appropriate to use an upper limit high enough to include the cross-section resonance but below all or most of the fission spectrum (which affects deviations from the 1/E flux weighting assumption). For an upper limit of 1 MeV, only 31% of the fission spectrum and almost all resonance peaks are included in the energy range.

With Eqs. (F7.6.16) and (F7.6.17) and the limits concluded above, the user can derive RES from flux groups 1 to m (denoting the range 0.5 eV to 1 MeV):

$$RES = \frac{1}{\ell n(E_2/E_1)} \sum_{i=1}^{m} \phi_i/\phi_{th} = 0.06892 \sum_{i=1}^{m} \phi_i/\phi_{th} \ . \qquad (F7.6.18)$$

FAST is applied in ORIGEN-S to those reactions, such as (n,α) and (n,2n), which have a threshold above 1 MeV. FAST is defined as 1.45 times the ratio of the flux above 1 MeV to the thermal flux. The user may apply a given flux spectrum in the manner similar to Eqs. (F7.6.12) and (F7.6.18) for the energy range above 1 MeV:

$$FAST = 1.45 \sum_{i=1}^{k} \phi_i/\phi_{th} \ . \qquad (F7.6.19)$$

F7.6.13 DATA NOTE C: (α,n) EMISSION IN BOROSILICATE GLASS

This data note discusses the methods for setting up a case that applies borosilicate glass in deriving (α,n) source strengths and neutron spectra.

Significant (α,n) emission rates and neutron spectra are produced in a material that contains sufficient quantities of α-emitters and light-element nuclei. A common example of neutron emission of this type is the neutron production from the (α,n) reactions with ^{17}O and ^{18}O in the UO_2 discharged from commercial reactors. The model applying (α,n) yields from UO_2 is the default in ORIGEN-S. There is interest, however, in computing the neutron source spectra produced from processed spent fuel (or high-level waste) contained in borosilicate glass. The model using data applicable to typical borosilicate glass is selected in ORIGEN-S when JOPT(11) = 1 is input in the 54$ data array.

Important differences are noted between the UO_2 and borosilicate glass models for producing (α,n) sources. The main purpose of this data note is to help the user understand that requirements for the borosilicate glass case are more extensive than those for the UO_2 case and the reasons for the additional input. The oxygen content may be input or may not be input to the UO_2 case. As long as JOPT(11) = 0 and JTO = 2, which are defaults (or JTO = 3 is input), the (α,n) source for UO_2 is computed without any additional changes to the problem input. However, it is important to note that the magnitudes of the (α,n) source strengths and spectra computed in cases using borosilicate glass are significantly dependent upon user input, other than setting the option triggers JOPT(11) and JTO.

A review of the description of the (α,n) model in Sect. F7.2.9 indicates the required input for the borosilicate glass case. Built-in spectral distributions (Table F7.2.2) are used for the four major α-emitters in high-level waste mixed with a specific borosilicate glass (Table F7.2.1). Then the combined spectral distribution, based upon (α,n) source strengths of the four major α-emitters, is normalized to the total (α,n) source strength of the entire mixture. It can be seen in Eqs. (F7.2.92) and (F7.2.93) that densities ρ_i of all isotopes or elements (or a constant times the densities) are applied. The densities of light elements are of primary importance because light elements tend to have significant (α,n) yields. However, the densities of heavier elements are also required because the magnitude of the (α,n) source is dependent on a weighting function that includes the α-stopping powers and densities of all elements in the material.

The input of the borosilicate glass case may follow descriptions referred to as either the "direct" or the "indirect" method of obtaining the material concentrations for the problem. The direct method applies only the concentrations input by the user in the 74* array. Even though this method is easier to understand, it can require considerably more of the user's time than the indirect method when exceedingly large numbers of

isotopes are to be input. For example, there could be hundreds of fission products and actinides in the high-level waste plus the elements in the borosilicate glass. However, if limited to a much smaller number of nuclides or elements, the case would require a more reasonable amount of the user's time.

There are different variations to the indirect method of deriving the required concentrations for the problem. One typical case using the indirect method is a problem in which reactor fuel is irradiated to a given burnup, cooled for a period, chemically separated as required to obtain high-level waste, mixed with borosilicate glass, and, finally, cooled for a time at which the neutron and photon spectra are required for dose rate evaluations. The indirect method involves the use of NOBLND in the 1$ data, FACT in the 2* array, and NGO and KBLEND in the 56$ array. Note that NOBLND is the "stream blending" trigger. Although the purpose of NOBLND implies the blending of material streams, it can be applied with equal effectiveness as a method of mixing two or more compositions. In simulating the typical case described earlier in this paragraph, the user should set up the input to compute the quantity of high-level waste and set NOBLND = 2, FACT(1) = 1, and FACT(2) = 1 in Data Blocks 1 and 2 of the case. Then, in the last subcase (producing the high-level waste), set NGO = −1 and KBLEND = MOUT (i.e., the last time step). Then, starting in Data Block 5, set up a decay-only subcase in which all of the borosilicate glass and all other elements that are to be mixed with the high-level waste are input. All elements must be converted to quantities such that the mass ratios between the fuel isotopes and the elements in the glass are correct. The case should be given a single time step and TIME(1) = 0, or a small value (e.g., 10^{-20} d). Also, set NGO = −1 and KBLEND = 1. Finally, set up a subsequent subcase to decay the mixture determined from the compositions of the two subcases in which KBLEND > 1. Required input to this subcase are KBLEND = −1 and JOPT(11) = 1, which flags the subcase as the one that applies the mixture produced from prior subcases using blending (i.e., KBLEND > 1), and applies the borosilicate glass (α,n) model. This completes the basic example of the indirect method of producing proper concentrations for the problem.

A variation to the previous example could be used to produce the source spectra (both neutron and photon) in the most convenient units of volume (e.g., cm^3). Use FACT(1) to convert the high-level waste to the proper units, because the first entry in FACT applies to the first blending subcase. Given that all of the computed high-level waste will be contained in V cm^3 of glass, set FACT(1) = 1/V. Then in the subcase in which borosilicate glass was input, use density units of g/cm^3 for each element and set FACT(2) = 1. If it is necessary to multiply the input by a factor, f, to convert to g/cm^3, set FACT(2) = f. The user should be aware that NN7 = 2 should be set in the last input of the 3$ data, which permits the input of composition in grams. When this is not the situation, change NGO = −1 to NGO = 0 in the subcase that computes the high-level waste, and start the borosilicate glass input case with the 3$ data and set NN7 = 2. In this case, never change library sizes from the earlier input sizes.

Other variations could be used in the computation of the high-level waste. Concentrations at some point in the calculation could be saved, either as unformatted data on NXTR (0$ array) using MOUT = 0 and MSUB > 0 (56$ array) or as formatted data on NPUN (56$ array) using JOPT(2) = 1 (54$ array). Then, in a later job, the case may be continued, compositions may be properly mixed, and the (α,n) source computed.

F7.7 SAMPLE CASES

Case 1 PWR Fuel Exposure and Decay

A scoping study is desired for a PWR, using the card-image ORIGEN-S library. Let the reactor operate at a power of 30 MW continually for 1100 days. List the complete inventory in gram-atoms per metric ton of uranium during both the exposure period and decay period. Also, list the results for the decay period in curies, total thermal power, the gamma source spectra (or "photon table results") produced by the input nuclear data library and the neutron source. Apply decay times of 10, 30, 60, 90, 120, 160, 270, 365, 1096, and 3652.5 days. List by nuclide only. The input concentrations are given in the data. Set THERM = 0.632, RES = 0.333, and FAST = 2. The input data follows:

```
=ORIGENS
0$$  A5  28  E  1$$  1  1T
PWR  NUCLEAR  DATA  -  SAMPLE CASE 1
4**  0.632  0.333  2  E  5$$  2  2T
35$$  0  4T
56$$  10  A13  50  4  3  0  2  1  E  57**  A3  1-14  E  5T
PWR - 3.3% ENRICHED U
  MT OF HEAVY METAL CHARGED TO REACTOR
58**  10R30  60**  81110  1100
66$$  1  A5  1  A9  1  E
73$$    60120   130270  140280  140290  220460  220470  220480  220490
220500  240500  240520  240530  240540  250550  260540  260560  260570  260580
270590  280580  280600  280610  280620  280640  400900  400910  400920  400940
400960  410930  420920  420940  420950  420960  420970  420980  421000  501120
501140  501150  501160  501170  501180  501190  501200  501220  501240
922350  922380  922340
74**   1.5  4.0   .607   .034   .304   .277  2.771  .204  .2  5.04
57.423  6.415  1.574  0.327  4.037   61.018  1.439  0.31  0.915  111.862
41.783  1.869  5.645  1.609  1421.122   306.725  462.239  460.074  72.5  10.258
0.957   .532   .926   .958   .546   1.357   .54   .321   .219   .113
4.681  2.47  7.729  2.739  10.392   1.467  1.823  140.4  4062  1.13
75$$   47R1   3R2   6T
56$$   0 10  A10  10  A17   2  E   5T
60**   10  30  60  90  120  160  270  365  1096  3652.5
65$$   1  5Z  1  2Z  1  11Z  1  5Z  1  2Z  1  11Z  1   5Z  1  2Z  1  E
61**  5R1-3  1+6  1+4
6T
56$$   F0   5T
END
```

(Job execution requires: 29 s on IBM 3090.)

Case 2 Time Integrated Fission Product Gamma Energy Spectra and Curies

Calculations are requested concerning fission product properties produced from exposing one gram of ^{235}U (as UO_2) to a thermal (or LWR) flux of 10^4 neutrons-cm^{-2} – s^{-1} for 1200 days in six intervals. Compute the time integral of the fission product gamma energy spectra and nuclides in Ci-s (with a cutoff of 10^{-30} Ci-s) over the first three months, the fourth month, and the thirteenth month. Apply: (1) $\sigma_f = 409$ barns for ^{235}U, which is in data set on unit 28 (and edit); (2) the binary mode Master Photon Library on unit 26; (3) either the utility submatrix data set for the integral option on unit 66, if available, or create it on unit 15; and (4) an energy group structure range of 0 – 11 MeV with the lowest two energy intervals input as $0 - 2 \times 10^5$, $2 \times 10^5 - 10^6$, and the remaining intervals of 10^6 eV for the spectra. The input data, making the submatrix data set, follows:

```
=ORIGENS
0$$ A5 28 A7 15 26 E 1$$ 1 1T
SAMPLE CASE 2 - LARGE FISSION PRODUCT LIBRARY
3$$ 28 A11 1 1 A16 2 A32 -15 12
4** 0.632 0.333 2 E 54$$ A9 2 E 2T
35$$ 0 4T
56$$ 6 6 1 A13 1 4 3 E 5T
U-235 FISSION PRODUCTS, SIGMA-F = 409 BARNS
 PER GRAM U-235 AT 10**4 N/(SEC-CM**2)
60** 4I 200 1200 73$$ 922350 74** 1 75$$ 2 59** F1+4 6T
56$$ 0 4 A10 6 A14 4 0 0 4 E 5T
60** 120 150 365.25 395.25 61** F1-30 65$$ A49 1 E
81$$ 2 0 26 1 E 82$$ 6 6 0 6 83** 9I 11+6 1+6 2+5 0 6T
GRAM U-235, 10**4 NEUTRONS/(SEC-CM**2), FIRST 3 MO. INTEGRAL SPECTRUM
GRAM U-235, 10**4 NEUTRONS/(SEC-CM**2), 4TH MO. INTEGRAL SPECTRUM
GRAM U-235, 10**4 NEUTRONS/(SEC-CM**2), 13TH MO. INTEGRAL SPECTRUM
56$$ F0 5T
END
```

(Job execution requires: 22 s on IBM 3090.)

F7.8 I/O UNIT ASSIGNMENTS

In addition to units for the libraries the user has selected along with the user card-image input and print units, the only (scratch) data set always required is on unit number NDISK. Also, if the user wishes to print FIDO edits on pages separate to the ORIGEN-S print, the use of unit NDUM is provided. The binary output units, NXTR, NVERT and LDSET, are required at the user's option. The following shows all logical units by name, default number, and purpose. Some of these are included in IBM mainframe procedures and workstation scripts.

UNIT	DEFAULT	PURPOSE
N5	5	Card input
KOUT	6	Printed output
NDUM	13	FIDO edits
NPUN	0	Card images of optional data saved
NDISK	11	Scratch
DECLIB	27	BCD ORIGEN-S decay data base
NDSET	28	BCD ORIGEN library input
NDSET	30	Binary ORIGEN library input
NVERT	0	Make or use in integral option
NDF	26	BCD photon data base input
NDF	26	Binary photon data base input
LDSET	51	Binary gamma source output
NXTR	0	Optional binary input/output unit
ND30	94	Binary problem data interface
|NGRP|	82	Neutron energy-group structure
|NG|	0	Photon energy-group structure

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APPENDIX F7.A

ORIGNATE User's Manual
PC Input Processor for ORIGEN-S

Stephen M. Bowman

F7.A.1 INTRODUCTION

ORIGNATE is a program designed to assist an ORIGEN-S user in preparing an input file for execution in SCALE-4. The program is written in Microsoft BASIC 7.1[31] and runs on an IBM- compatible personal computer and produces a card-image input file that may be uploaded to a mainframe computer to execute ORIGEN-S in SCALE-4. ORIGNATE features a pulldown menu system with sophisticated data entry screens containing context-sensitive help messages, which were designed with QuickScreen[32] and QuickPak Professional[33] from Crescent Software. The menu system organizes the major command categories as menu titles and pulldown commands. The program performs extensive error checking for each input screen and presents warning and error message boxes and yes/no dialog boxes to verify that the user wants to perform certain functions (e.g., write over files which have been saved previously). The menus may be used with either a keyboard or a mouse.

F7.A.2 GETTING STARTED

To install ORIGNATE, first make a directory on your hard disk where ORIGNATE will reside by using the DOS MKDIR command:

```
MKDIR \ORIGNATE
```

Next, change to that directory:

```
CHDIR \ORIGNATE
```

Then place the ORIGNATE distribution diskette into drive A (or other drive of your choice):

```
COPY A:\ORIGNATE\*.*
```

This will install all the ORIGNATE files. To execute the program, enter the program name:

```
ORIGNATE
```

Now you are ready to start. The easiest way to learn how to use ORIGNATE is to read through the rest of the documentation while you are running the program so you can use the options and keys as you read about them. The following two sections, "Using the Menu System" and "Using the Input Screens" give an overview of how to use the program. Following those sections is a detailed description of how to use each of the menu options.

F7.A.3 USING THE MENU SYSTEM

After paging through the introductory screen, you reach the ORIGNATE pulldown menu system. The menu system contains a menu bar across the top of the screen. Under each menu bar option there is a unique pulldown menu. The menu bar options are summarized below.

Files	Options to retrieve files, save files and exit the program
Initial Input	Options to input compositions and energy group edit structure

Case Types	Options to input depletion cases and decay cases
Modifying Cases	Options to insert cases and delete cases

When ORIGNATE begins, it presents the **Files** pulldown menu. You may scan across the menu bar by using the left and right arrow keys. You may select an option from a pulldown menu by using the up and down arrow keys. A description of the highlighted option will appear on the bottom line of the screen. To execute the option, simply press the <Enter> key or the highlighted letter (known as the "hot key") of the desired option.

The mouse may also be used to select an option by moving it left or right along the menu bar or up and down on a pulldown menu. To choose a pulldown menu command, simply move the mouse cursor over the desired option and click the left mouse button. Some users may prefer to "drag" the mouse (holding the left mouse button) over the menus and then release the left button when the cursor is over the desired command. One difference between the two methods of using the mouse is that dragging the mouse will cause the description of the highlighted option to be displayed on the bottom of the screen as when using the keyboard.

Some pulldown menu commands are black with a hot key while others are gray. The black commands are active; the gray commands are inactive and will produce no effect if selected. Commands will be activated as necessary data are entered. For example, once the Initial Input data are entered, the Case Types options are active. Most of the options will become active when ORIGNATE files are retrieved.

F7.A.4 USING THE INPUT SCREENS

Once an option is selected, an input screen or series of input screens will be displayed. The cursor will appear at the first data field on the screen which is not protected. Fields may be protected by the program depending on the input options selected. For example, on the Compositions screen, if "Input" is "Dataset", the nuclide fields for card input are protected. To move from one field to the next, press <Enter> or <Tab>. To move backward to the previous field, press <Shift+Tab> or <Backspace>. The cursor must be at the beginning of the field for <Backspace> to move to the previous field, because within a data field it moves back one space and deletes the previous character. You may also change fields with the arrow keys, but the movement will be somewhat erratic as the cursor skips fields if there is more than one field per screen line. <Home> moves the cursor to the beginning of the field, and <End> moves to the end of the field. The <Ins> and <Del> keys perform their normal functions for editing a field. <Ctrl+Home> moves the cursor to the first field on the screen, and <Ctrl+End> moves the cursor to the last field. <PgUp> and <PgDn> may perform the same respective functions, if they are not active functions listed on the bottom of the current input screen.

Some fields have a multiple choice menu associated with them. Pressing <Enter> or the Space Bar at one of these fields will activate the multiple-choice menu. When this menu is displayed, all other processing and function keys are disabled until a choice is selected and the menu disappears from the screen. Pressing a letter on the keyboard will move the cursor to the next choice that begins with that letter. If there is not a choice which begins with that letter, the cursor moves to the beginning of the list. The up and down arrow keys, <PgUp>, <PgDn>, or the mouse may be used to make a selection. <Home> moves the cursor to the first choice, and <End> moves the cursor to the last choice. Once the desired choice is highlighted, press <Enter> to select it and remove the menu.

Logical (YES or NO) fields use "Y" and "N" or "X" and " ". No other values will be accepted. You may toggle between the two choices with the space bar.

Most fields have a help message associated with them. Pressing <F1> displays the message. Often the message will refer to a section of the SCALE manual for more detailed information. Press <Enter> or

<Esc> to remove the message from the screen. If there is no message for a particular field and it is one of several identical fields on a screen, try moving the cursor to the first of these fields on the screen and pressing <F1>. For the Compositions screens, the help messages are only active for the first screen and the first occurrence of each field on subsequent screens.

Title and comment fields must be entered whenever they appear on an input screen. Delimiters are automatically provided by ORIGNATE and should not be input by the user.

F7.A.5 MENU SYSTEM OPTIONS

The purpose of this section is to present an overview of the menu system commands. Menu bar options are presented next to square bullets; corresponding pulldown commands are listed next to round bullets. The underlined letter in commands discussed below represents the hot key for the command; these hot keys appear on screen as bright letters, and they allow immediate access to an item by pressing the highlighted key.

■ *Files*

The **Files** menu allows you to retrieve and save files and to exit the program.

- **Retrieve Files**

This option allows you to retrieve random access files which you have previously saved with ORIGNATE. A random access file is saved for each pulldown menu option for which data are entered. Each random access file for a problem has the same file name as specified by the user but a different file extension designated by ORIGNATE. A listing of these file extensions is given in Table F7.A.1. ORIGNATE presents a list of all files in the current directory that have the ".CMP" file extension (this random access file is always required). When you select the desired file name, ORIGNATE loads all files with that file name and one of the extensions listed in Table F7.A.1. The program copies the files to a set of temporary files, ORIGTEMP.* (i.e., file extensions remain the same). If you wish to retrieve only a portion of the ORIGNATE files associated with an ORIGEN-S input file you have previously generated (e.g., the Compositions data), rename or copy those files using the same file extensions. Two sets of sample files have been provided on the distribution diskette. The naming conventions are BWR.* and PWR.* and represent actual BWR and PWR fuel assembly depletions, respectively. These sample problems are discussed in detail in the final section of this manual.

Table F7.A.1 ORIGNATE random access files

ORIGNATE file extensions	Contents
.CMP	Compositions input
.DCY	Decay cases
.DPL	Depletion cases
.GRP	Energy group structures

- **Save Files / Input Deck**

This option saves the data you have entered in random-access files, which can later be retrieved by the program for modification. A card image ORIGEN-S input file is also generated. ORIGNATE will not save files in this option unless sufficient data have been entered to generate a meaningful ORIGEN-S input file. A random-access file will be saved for each menu option used to input data, up to a maximum of four files. ORIGNATE will prompt you for the file name for the ORIGNATE files and the file name and the extension for the card image ORIGEN-S input file. If files with these names already exist, ORIGNATE will ask if you want to overwrite these files. You also have the option of having ORIGNATE generate job control language (JCL) for your ORIGEN-S input file. ORIGNATE reads an ASCII text dataset JCLNAMES.DAT to obtain the default dataset name prefixes for the JCL. This allows an IBM user at sites other than Oak Ridge Naitonal Laboratory to be able to use this feature. ORIGNATE allows the use of two types of depletion libraries, SCALE supplied (libraries supplied with SCALE-4.1) and user supplied (previously generated by the user with SAS2). The JCLNAMES.DAT file contains default values for both, as shown in Table F7.A.2.

Table F7.A.2 JCLNAMES.DAT input description

Line	Variable	Maximum Length	Description
1	Library1$	5	First prefix for SCALE-supplied libraries
2	Library2$	8	Second prefix for SCALE-supplied libraries
3	Other1$	5	First prefix for user-supplied libraries
4	Other2$	8	Second prefix for user-supplied libraries
5	Other3$	8	Third prefix for user-supplied libraries

- **Save Partial Files**

This option saves ORIGNATE random-access files, regardless of the amount of data entered. It does not generate a card image ORIGEN-S input file. This option is designed to allow you to occasionally save input data so that it will not be lost if the program terminates abnormally. Note that if ORIGNATE does fail, the data entered still exist in the ORIGTEMP.* files. When ORIGNATE is restored, it will notify you that it has detected these files and will give you an opportunity to rename and save them.

- **Quit**

This option terminates the program. If you have selected any option other than retrieving or saving files immediately prior to this option, the program will verify if this is what you want to do. Since this option does not save files, you may also use this option to cancel any changes you have made since the last time you saved files.

■ *Initial Input*

The **Initial Input** menu provides you with selections to input the case independent initial data required by ORIGEN-S.

• **Compositions**

This option is the only active option other than Retrieve Files when you enter the program. Select either "Cards" or "Dataset" as your source of input in the first field. If "Cards" is selected, the second field gives you a choice of input units. You specify each nuclide by element from an alphabetized menu and then type the isotope (e.g., "U(92)" and "235" for U-235 and "Xe(54)" and "135m" for Xe-135 metastable). The program checks the isotope number to ensure it is valid for the element selected. A complete list of valid isotopes is given in Appendix B. To obtain the natural abundances of an element in the ORIGEN-S light element library (NEX1=4 in the ORIGEN-S 75$ array), input "Natl" for the isotope. If the specified nuclide appears in more than one of the ORIGEN-S master libraries (light element, actinide, or fission product), a menu is provided of the available libraries. Select a library based on the origin of the nuclide and the desired edit grouping. If only one library is valid, the program automatically fills the field with the appropriate library. Then input the concentration in the units previously selected. The concentration that is input for each nuclide determines the "basis" of the problem (e.g., fuel assembly, metric ton of uranium, etc.)

This option displays a maximum of three screens. Each screen contains ten nuclides, for a maximum of 30 nuclides. The <PgDn> and <PgUp> keys are used to move forward and backward, respectively, between screens. To change an element selection, simply select a new one from the multiple-choice menu. To erase an element which has been selected, press <Ctrl+E> while the cursor is on that element field.

If you want ORIGEN-S to read the nuclides from a dataset written by a previous ORIGEN-S job, select "Dataset" as the source of input in the first field. All nuclide fields are then blanked and protected. The second field then represents the I/O unit number of the dataset and the position of the concentrations in the dataset. For example, "71+2" specifies I/O unit No. 71 and the second position in the file. Note that ORIGEN-S prints the position in the file when it writes the data. If you omit the position number from this field, ORIGNATE assumes that you want to read from the first position in the file.

IMPORTANT NOTE: If you read and write restart data in the same job, ORIGEN-S begins writing data in the file position immediately following the one from which it read. It does not search for the end of file. **If you are reading from a position prior to the last one in the file, the data which follows may be overwritten if new restart data are saved.**

Use <F4> to cancel or <F10> to save the data and return to the main menu.

• **Neutron/Gamma Groups**

This option displays two screens, one each for the energy group structure for neutron spectra edits and gamma spectra edits. These edits are for individually selected time steps in the decay cases. The first field on each screen gives a multiple choice list of energy group structures corresponding to commonly used neutron or gamma cross section libraries. You may choose one of these or input your own group structure by selecting "Other". If you are running only depletion cases or you do not want these edits, you may select "None".

If you select one of the standard group structures or "None", ORIGNATE protects the remaining fields on the screen and advances to the next screen. <PgUp> and <PgDn> may be used to move from one screen to the other. If you select "Other", specify the number of energy groups. ORIGNATE requires you to input the maximum energy cutoff in eV for each group, beginning with group 1 (the highest energy group). The field following the maximum energy cutoff for the lowest energy group must contain the minimum energy cutoff for that group. The remaining fields on the page remain protected. ORIGNATE verifies that the energies are entered in order from highest to lowest.

■ Case Types

The **Case Types** menu provides you with selections to enter depletion and/or decay case data. (A "case" in ORIGNATE is equivalent to a "subcase" in ORIGEN-S.) Each case is limited to ten time steps, because this is the maximum number that fit across a page of the ORIGEN-S output. Each case has a title card and a basis card. The basis card is a subtitle in the ORIGEN-S output that describes the basis for the calculations performed as determined by the concentrations input (e.g., a fuel assembly, or a metric ton of uranium). All depletion cases are entered via one option, and all decay cases are entered via another option. The order in which they are entered determines the order in which they appear in the ORIGEN-S input file and is reflected by the case number which is displayed in ORIGNATE.

• Depletion Cases

This option displays three screens: (1) the depletion case input, (2) the depletion case I/O options, and (3) the depletion case library specifications. The screen initially displayed is the depletion case input for a new case with a case number one greater than the last case saved. The data for a case are saved by pressing <F10> to advance to the next case, or <F9> to go back to the previous case. To avoid saving changes on the screen, press <F4> to return to the main menu system. ORIGNATE asks you if you want to save the changes on the screen before returning. To review existing cases, press <Ctrl+R>. This displays a list of case numbers, types, and titles.

Each depletion case consists of a series of time steps. The beginning time, which is defaulted to zero, and the ending time for the case are specified first. Then the power (MW / basis unit) and the cumulative time from the case beginning time are input for each time step.

IMPORTANT NOTE: The power must be consistent with the basis for the calculation (e.g., fuel assembly, MTU, etc.).

To specify downtime during or at the end of the case, input 0 for the power. (ORIGNATE automatically resets it to 1.0E-20.) For periods greater than 100 days, a separate decay case is recommended. The time entered for the last time step must match the "ending time" field. In addition, the program checks that the cumulative time for each step is greater than the previous step. The maximum recommended increment per time step is 100 days or 0.3 years, and the recommended minimum number of steps is three per case. If the time step increments are larger or the number of time steps is less, ORIGNATE prints a message on the screen and automatically inserts additional steps up to the maximum of ten steps per case. The intent of this feature is to allow you to specify only the times at which you want to change power level or obtain output and let ORIGNATE determine any remaining steps needed to ensure accurate results. You can modify the steps generated by ORIGNATE by simply editing the fields. ORIGNATE only checks the data once per edit of each case. If you later return to a case and edit any of the data, ORIGNATE checks the length and number of time steps again.

The option to write restart data for a time step is set by typing an "X" in the appropriate field. These data may be written for as many time steps as desired. If the compositions input specified reading from a dataset, these data are written to the same unit, immediately following the input data read. As noted previously, **this will result in a loss of any data following the input data in that dataset.** If the compositions input was specified on cards, the restart data is written to I/O unit 71.

The I/O options screen is accessed by pressing <Ctrl+O>. This screen only controls the I/O options for depletion cases. This screen must be edited and saved for the first depletion case. ORIGNATE

automatically displays it with a set of default values when you press <F10> to initially save the first case. The options stay in effect until they are changed in a subsequent case. The time units that are displayed on the depletion case input screen are selected on this screen.

The library options screen is used to specify the binary depletion library for each case. Note that ORIGNATE is not designed for use with card image libraries, but only binary libraries. The ORIGEN-S card image libraries contain data that are only suitable for general scoping calculations. Although it is recommended that more appropriate binary libraries be used, the PRLIMLWR binary library is available in SCALE-4 (see Section M6.7.3 of the SCALE-4 manual). It is a modified version of the ORIGEN-S card image libraries.

The library options screen is accessed by pressing <Ctrl+L>. This screen specifies the binary ORIGNATE automatically displays the library options screen with the values from the previous case when you press <F9> or <F10> to initially save a new case. It is very important that you choose an appropriate library for each case. In order to ensure that this is done, ORIGNATE requires that you edit this screen for each case. If you use the same library for consecutive cases, the program prints a dialog box to verify that you want to do that. You have the option of specifying the I/O unit number and position in the file for a user-supplied library which has been previously generated with SAS2 or selecting one of the SCALE supplied libraries (available in SCALE-4.1 or later). The SCALE supplied libraries are categorized by:

(1) reactor type,
(2) enrichment / maximum burnup,
(3) power, and
(4) cycle number / burnup range.

The selections available for each of these are shown in Table F7.A.3. The nearest enrichment should be the criterion for choosing the enrichment / maximum burnup. The maximum burnup is simply an upper bound for which cross sections are available. The burnup range is the criterion for selecting the cycle number / burnup range. The cycle number is an arbitrary indexing for the libraries generated for a particular enrichment and does not necessarily correspond to the number of cycles in which the fuel being modeled has been burned. An ORIGNATE case that exceeds the lower or upper burnup limit by 5 or 10% is acceptable. For some fuel cycles, it may be necessary to break up the cycle into two or more cases to match the burnup ranges of the depletion libraries. An example would be a 3.6 wt% PWR fuel assembly that accumulates 18 GWd/MTU of burnup in its first cycle. This would require one case from 0 to 10 GWd/MTU and a second from 10 to 18 GWd/MTU. The first case would use the Cycle 1 / 0 - 10 GWd/MTU library, and the second would use the Cycle 2 / 10 - 20 GWd/MTU library.

The I/O unit numbers for the SCALE libraries are automatically assigned beginning with unit 51. For user-supplied libraries, you may use unit numbers between 31 and 50 in order to avoid conflicts with other SCALE datasets. You must ensure that your job control language specifies the correct dataset names for the libraries you use, whether they are SCALE or user supplied libraries.

- **Decay Cases**

This option displays three screens: (1) the decay case input, (2) the decay case I/O options, and (3) element fractions. The screen initially displayed is the decay case input for a new case with a case number one greater than the last case saved. The <F4>, <F9>, <F10>, and <Ctrl+R> keys function the same as on the depletion case input screen.

Like a depletion case, each decay case consists of a series of time steps. The beginning time, which is defaulted to zero, and the ending time for the case are specified first. The time entered for the last time step

Table F7.A.3 SCALE-supplied library parameters

Reactor Type: PWR

	Power (MW/MTU)	
	18	
28		
	40	

Enrichment / Maximum Burnup (wt % U-235)	(GWd/MTU)	Number of Cycles	Burnup per Cycle (GWd/MTU)
2.4 wt% /	25	3	8.333
2.8 wt% /	30	3	10.000
3.2 wt% /	35	4	8.750
3.6 wt% /	40	4	10.000
3.9 wt% /	45	5	9.000
4.2 wt% /	50	5	10.000

Reactor Type: BWR

	Power (MW/MTU)	
	12	
20		
	30	

Enrichment / Maximum Burnup (wt % U-235)	(GWd/MTU)	Number of Cycles	Burnup per Cycle (GWd/MTU)
1.9 wt% /	20	3	6.667
2.3 wt% /	25	3	8.333
2.7 wt% /	30	4	7.500
3.1 wt% /	35	4	8.750
3.4 wt% /	40	5	8.000
3.8 wt% /	45	5	9.000

must match the "ending time" field. In addition, the program checks that the cumulative time for each step is greater than the previous step. The recommended maximum initial time step is 100 days or 0.3 years, and the cumulative time for subsequent steps should be ≤ 3.3 times the cumulative time for the previous time step. Because the nuclides decay exponentially, this factor ensures accurate results. This is commonly known as the "Rule of 3's". If the time step increments are larger, ORIGNATE prints a message on the screen and automatically inserts additional steps up to the maximum of ten steps per case. For a cumulative time of 3 raised to a power of 10 (0.3, 3, 30, 300, etc.), ORIGNATE sets the time for the next step to 10 raised to the same power of 10 (1, 10, 100, 1000, etc.). The intent of this feature is to allow you to specify only the times at which you want to obtain output and let ORIGNATE determine any remaining steps needed to ensure accurate results. You can modify the steps generated by ORIGNATE by simply editing the fields. ORIGNATE only checks the data once per edit of each case. If you later return to a case and edit any of the data, ORIGNATE checks the length and number of time steps again.

The decay case input screen allows you to save restart file data in the same manner as the depletion case input screen. In addition, it allows you to request neutron and gamma source spectra output edits for any time step. These are printed by ORIGEN-S according to the energy group structures designated in the Neutron/Gamma Groups option. If "None" is selected for both group structures, requesting an edit on this screen has no effect.

The I/O options screen is accessed by pressing <Ctrl+O>. This screen only controls the I/O options for decay cases. This screen must be edited and saved for the first decay case. ORIGNATE automatically displays it with a set of default values when you press <F10> to initially save the first case. The options stay in effect until they are changed in a subsequent case. The time units which are displayed on the decay case input screen are selected on this screen. The (α,n) source is typically UO_2, unless you are modeling high-level waste in borosilicate glass. See Sects. F7.2.8 and F7.2.9 of the SCALE manual for details. ORIGEN-S allows the cutoff for the decay output edits to be in the units of the edit or % of the total. The latter is designated by typing "%" at the end of the cutoff value. In order to simplify the output edits menu, the 63 choices possible in the ORIGEN-S 65$ array (see Sect. F7.6.10) have been reduced by grouping according to the three dimensions of the array. This may result in more output than desired in some cases (e.g., in some cases only grams of light elements but grams and curies of fission products). The ORIGEN-S card image input generated by ORIGNATE has been formatted and labeled by subgroups so that an experienced ORIGEN-S user can easily modify the input by turning on or off individual edit options in the 65$ array.

The element fractions screen is an optional screen that allows you to keep or remove all or part of a maximum of ten elements from the previous case. This allows you to isolate part of the problem being modeled, such as the endfittings of a fuel assembly. To access this screen, type "Y" for the element fractions field on the decay case input screen and press <Ctrl+F>. Select whether you want to keep or remove the elements, then select the elements from a multiple choice menu, and specify the fractions of each to be kept or removed.

- **Review Cases**

This option displays a list of case numbers, types, and titles for all cases which have been created. This function may also be performed by pressing <Ctrl+R> at the main menu or while using screens which require case numbers: Depletion Cases (screen 1) and Decay Cases. To remove the list from the screen, press <Enter> or <Esc>.

■ *Modifying Cases*

The **Modifying Cases** menu contains options for inserting or deleting cases, so that you can retrieve an existing set of cases and modify them to model different scenarios, such as adding or deleting a cycle from a fuel assembly's burnup history.

- **Insert Cases**

This option presents a dialog box with two fields: the type of case to be inserted (depletion or decay), and where to insert it (the new case goes before the case selected). Use the <Tab> and <Shift+Tab> keys to move between the two fields and the up and down arrow keys to select the choice for each field. The mouse may also be used in the dialog box. Selecting the <Cancel> button at the bottom of the box or pressing <Esc> returns you the main menu system without inserting a case. When you press <Enter> or click the

mouse to accept the choices made, ORIGNATE automatically adjusts the case numbers and takes you directly to the depletion or decay input screen to enter the data for the new case.

- **Delete Cases**

This option presents a dialog box with a list of all cases. Select the case to delete by using the up and down arrow keys or the mouse. The case numbers for the remaining cases will be automatically adjusted. Selecting the <Cancel> button at the bottom of the box or pressing <Esc> returns you the main menu system without deleting a case.

F7.A.6 FILES ON THE DISTRIBUTION DISKETTE

Files included on the ORIGNATE distribution diskette which are necessary for running the program are listed in Table F7.A.4. ORIGNATE.EXE is the executable program. ORIGNATE.QSL is the ORIGNATE QuickScreen Library developed with Crescent Software's QuickScreen program. This library contains all the input screens displayed by ORIGNATE. The files with the ".FRM" extension contain the form definition for each of the screens in the library. The files with the ".BSV" extension were written with Microsoft BASIC's BSAVE command and contain the following data: nuclides, elements, neutron energy group boundaries, and gamma group energy group boundaries.

In addition to these files, ORIGNATE files for a sample BWR and a sample PWR problem are included on the diskette. These files are listed in Table F7.A.5. You may retrieve them in ORIGNATE. The card image ORIGEN-S input files that were generated with these files have the extension ".IN". The BWR case models assembly CZ205 from Cooper Nuclear Station. This assembly was in core for three cycles, out of core for two cycles, and in core for two more cycles.

The PWR case models assembly D-15 from Turkey Point Unit 3. This assembly was used for three consecutive cycles and then discharged. The power histories and other pertinent data for these two assemblies used in setting up the ORIGNATE input data are presented in Tables F7.A.6, F7.A.7, and F7.A.8. These two assemblies have been used for decay heat measurements which have served as benchmarks for ORIGEN-S calculations. For more information, see ref. 34.

Finally, a copy of this document is included on the diskette in the README.DOC file.

Table F7.A.4 Files required by ORIGNATE

File name	Extension
COMPNUC1	.FRM
COMPNUC2	.FRM
DECACAS1	.FRM
DECACAS2	.FRM
DECACAS3	.FRM
DEPLCAS1	.FRM
DEPLCAS2	.FRM
DEPLCAS3	.FRM
G18ORIG2	.BSV
G18SCALE	.BSV
G20	.BSV
G44	.BSV
GROUP1	.FRM
GROUP2	.FRM
N218	.BSV
N22	.BSV
N227	.BSV
N238	.BSV
N27	.BSV
N47	.BSV
ORIGCOMP	.BSV
ORIGELEM	.BSV
ORIGNATE	.EXE
ORIGNATE	.QSL
RENAMFIL	.FRM
SAVEFIL	.FRM
SAVEPART	.FRM

Table F7.A.5 ORIGNATE sample problem files

File names	
BWR.CMP	BWR sample problem
BWR.DCY	
BWR.DPL	
BWR.GRP	
BWR.JCL	PWR sample problem
BWR.OUT	
PWR.CMP	
PWR.DCY	
PWR.DPL	
PWR.GRP	
PWR.JCL	
PWR.OUT	

Table F7.A.6 Data for Cooper BWR Assembly CZ205

Burnup History Data

Cycle No.	Power (MW/ass'y)	Burnup (MWd/MTU)	Cycle length (days)	Outage length (days)
1	2.427	10,298	807	59
2	4.608	7,414	306	31
3	3.464	2,987	164	35
4[a]	0.0	0	370	--
5[a]	0.0	0	394	--
6	1.118	1,864	317	48
7	1.520	2,781	348	--
Total		25,344	1942	

[a]Assembly was out of core during this cycle

Average power = 25,344 MWd/MTU / 1942 days = 13.05 MW/MTU

Fuel loading = 0.1902 MTU
Initial uranium isotopics: ^{234}U wt % = 0.022 ^{235}U wt % = 2.500
^{236}U wt % = 0.012 ^{238}U wt % = 97.466

Cooling times (days): 857 871 886 892 899 946
Measured heat (watts): 324.0 343.5 331.8 327.5 311.4 317.1

Table F7.A.7 Data for Turkey Point 3 PWR Assembly D-15

Burnup History Data

Cycle No.	Power (MW/ass'y)	Burnup (MWd/MTU)	Cycle length (days)	Outage length (days)
2	13.771	9,480	314	58
3	13.603	9,752	327	62
4	13.040	8,920	312	--
Total			28,152	953

Average power = 28,152 MWd/MTU / 953 days = 29.54 MW/MTU

Fuel loading = 0.4561 MTU
Initial uranium isotopics: ^{234}U wt % = 0.023 ^{235}U wt % = 2.557
^{236}U wt % = 0.012 ^{238}U wt % = 97.408

Cooling times (days): 962 1144 2077
Measured heat (watts): 1423 1126 625

Table F7.A.8. Fuel assembly light-element contents

Element	Cooper Station (kg/assembly)	Turkey Point (kg/assembly)
H	3.1000	---
B	0.0130	---
O	50.5000	62.000
Cr	0.4500	2.700
Mn	0.0290	0.150
Fe	1.2000	5.900
Co	0.0046	0.034
Ni	0.4500	4.500
Zr	98.2000	101.000
Nb	---	0.320
Sn	1.6000	1.600
Gd	0.5440	---

APPENDIX F7.B

ORIGEN-S Nuclides

Table F7.B.1 ORIGEN-S light elements

H-1	Al-27	Ca-48	Ni-58	Se-74
H-2	Al-28	Ca-49	Ni-59	Se-75
H-3	Al-29	Sc-45	Ni-60	Se-76
H-4[a]	Al-30	Sc-46	Ni-61	Se-77
He-3	Si-28	Sc-46m	Ni-62	Se-77m
He-4	Si-29	Sc-47	Ni-63	Se-78
He-6	Si-30	Sc-48	Ni-64	Se-79
Li-6	Si-31	Sc-49	Ni-65	Se-79m
Li-7	Si-32	Sc-50	Ni-66	Se-80
Li-8	P-31	Ti-46	Cu-62	Se-81
Be-8	P-32	Ti-47	Cu-63	Se-81m
Be-9	P-33	Ti-48	Cu-64	Se-82
Be-10	P-34	Ti-49	Cu-65	Se-83
Be-11	S-32	Ti-50	Cu-66	Se-83m
B-10	S-33	Ti-51	Cu-67	Br-79
B-11	S-34	V-49	Zn-63	Br-80
B-12	S-35	V-50	Zn-64	Br-80m
C-12	S-36	V-51	Zn-65	Br-81
C-13	S-37	V-52	Zn-66	Br-82
C-14	Cl-35	V-53	Zn-67	Br-82m
C-15	Cl-36	V-54	Zn-68	Br-83
N-13	Cl-37	Cr-50	Zn-69	Kr-78
N-14	Cl-38	Cr-51	Zn-69m	Kr-79
N-15	Cl-38m	Cr-52	Zn-70	Kr-79m
N-16	Ar-36	Cr-53	Zn-71	Kr-80
O-16	Ar-37	Cr-54	Zn-71m	Kr-81
O-17	Ar-38	Cr-55	Ga-69	Kr-81m
O-18	Ar-39	Mn-54	Ga-70	Kr-82
O-19	Ar-40	Mn-55	Ga-71	Kr-83
F-19	Ar-41	Mn-56	Ga-72	Kr-83m
F-20	Ar-42	Mn-57	Ga-72m	Kr-84
Ne-20	K-39	Mn-58	Ge-70	Kr-85
Ne-21	K-40	Fe-54	Ge-71	Kr-85m
Ne-22	K-41	Fe-55	Ge-71m	Kr-86
Ne-23	K-42	Fe-56	Ge-72	Kr-87
Na-22	K-43	Fe-57	Ge-73	Kr-88
Na-23	K-44	Fe-58	Ge-74	Rb-85
Na-24	Ca-40	Fe-59	Ge-75	Rb-86
Na-24m	Ca-41	Co-58m	Ge-75m	Rb-86m
Na-25	Ca-42	Co-58	Ge-76	Rb-87
Mg-24	Ca-43	Co-59	Ge-77	Rb-88
Mg-25	Ca-44	Co-60	Ge-77m	Rb-89
Mg-26	Ca-45	Co-60m	As-75	Sr-84
Mg-27	Ca-46	Co-61	As-76	Sr-85
Mg-28	Ca-47	Co-62	As-77	Sr-85m

Table F7.B.1 (continued)

Sr-86	Mo-98	Ag-107	Sn-113m	I-125
Sr-87	Mo-99	Ag-108	Sn-114	I-126
Sr-87m	Mo-100	Ag-108m	Sn-115	I-127
Sr-88	Mo-101	Ag-109	Sn-116	I-128
Sr-89	Tc-97	Ag-109m	Sn-117	I-129
Sr-90	Tc-97m	Ag-110	Sn-117m	I-130
Sr-91	Tc-98	Ag-110m	Sn-118	I-130m
Sr-93	Tc-99	Ag-111	Sn-119	I-131
Y-89	Tc-100	Ag-111m	Sn-119m	I-132
Y-89m	Tc-101	Ag-112	Sn-120	Xe-124
Y-90	Ru-96	Cd-106	Sn-121	Xe-125
Y-90m	Ru-97	Cd-107	Sn-121m	Xe-125m
Y-91	Ru-98	Cd-108	Sn-122	Xe-126
Y-92	Ru-99	Cd-109	Sn-123	Xe-127
Y-93	Ru-100	Cd-110	Sn-123m	Xe-127m
Y-94	Ru-101	Cd-111	Sn-124	Xe-128
Y-96	Ru-102	Cd-111m	Sn-125	Xe-129
Zr-89	Ru-103	Cd-112	Sn-125m	Xe-129m
Zr-90	Ru-104	Cd-113	Sb-121	Xe-130
Zr-91	Ru-105	Cd-113m	Sb-122	Xe-131
Zr-92	Ru-106	Cd-114	Sb-122m	Xe-131m
Zr-93	Ru-107	Cd-115	Sb-123	Xe-132
Zr-94	Rh-102	Cd-115m	Sb-124	Xe-133
Zr-95	Rh-103	Cd-116	Sb-124m	Xe-133m
Zr-96	Rh-104	Cd-117	Sb-125	Xe-134
Zr-97	Rh-104m	Cd-117m	Sb-126	Xe-135
Nb-91	Rh-105	Cd-119	Sb-126m	Xe-135m
Nb-92	Rh-105m	Cd-121	Te-120	Xe-136
Nb-93	Rh-106	In-113	Te-121	Xe-137
Nb-93m	Rh-106m	In-113m	Te-121m	Cs-131
Nb-94	Rh-107	In-114	Te-122	Cs-132
Nb-95	Pd-102	In-114m	Te-123	Cs-133
Nb-95m	Pd-103	In-115	Te-123m	Cs-134
Nb-96	Pd-104	In-116	Te-124	Cs-134m
Nb-97	Pd-105	In-116m	Te-125	Cs-135
Nb-97m	Pd-106	In-117	Te-125m	Cs-136
Nb-98	Pd-107	In-117m	Te-126	Cs-137
Nb-100	Pd-107m	In-118	Te-127	Cs-138
Mo-92	Pd-108	In-119	Te-127m	Ba-130
Mo-93m	Pd-109	In-119m	Te-128	Ba-131
Mo-93	Pd-109m	In-120	Te-129	Ba-131m
Mo-94	Pd-110	In-120m	Te-129m	Ba-132
Mo-95	Pd-111	In-121	Te-130	Ba-133
Mo-96	Pd-111m	Sn-112	Te-131	Ba-133m
Mo-97	Ag-106	Sn-113	Te-131m	Ba-134

Table F7.B.1 (continued)

Ba-135	Pm-150	Dy-165	Hf-179	Ir-194m
Ba-135m	Pm-151	Dy-165m	Hf-179m	Pt-190
Ba-136	Pm-152	Dy-166	Hf-180	Pt-191
Ba-136m	Sm-144	Ho-163	Hf-180m	Pt-192
Ba-137	Sm-145	Ho-165	Hf-181	Pt-193
Ba-137m	Sm-146	Ho-166	Hf-182	Pt-193m
Ba-138	Sm-147	Ho-166m	Ta-180	Pt-194
Ba-139	Sm-148	Er-162	Ta-181	Pt-195
Ba-140	Sm-149	Er-163	Ta-182	Pt-195m
Ba-141	Sm-150	Er-164	Ta-182m	Pt-196
La-137	Sm-151	Er-165	Ta-183	Pt-197
La-138	Sm-152	Er-166	W-180	Pt-197m
La-139	Sm-153	Er-167	W-181	Pt-198
La-140	Sm-154	Er-167m	W-182	Pt-199
La-141	Sm-155	Er-168	W-183m	Pt-199m
Ce-136	Eu-151	Er-169	W-183	Au-197
Ce-137	Eu-152	Er-170	W-184	Au-198
Ce-137m	Eu-152m	Er-171	W-185	Au-199
Ce-138	Eu-153	Er-172	W-185m	Au-200
Ce-139	Eu-154	Tm-169	W-186	Hg-196
Ce-139m	Eu-155	Tm-170	W-187	Hg-197
Ce-140	Eu-156	Tm-170m	W-188	Hg-197m
Ce-141	Gd-152	Tm-171	W-189	Hg-198
Ce-142	Gd-153	Tm-172	Re-185	Hg-199
Ce-143	Gd-154	Tm-173	Re-186	Hg-199m
Ce-144	Gd-155m[a]	Yb-168	Re-187	Hg-200
Ce-145	Gd-155	Yb-169	Re-188	Hg-201
Pr-141	Gd-156	Yb-170	Re-188m	Hg-202
Pr-142	Gd-157	Yb-171	Re-189	Hg-203
Pr-142m	Gd-158	Yb-172	Os-184	Hg-205
Pr-143	Gd-159	Yb-173	Os-185	Tl-203
Pr-144	Gd-160	Yb-174	Os-186	Tl-204
Pr-145	Gd-161	Yb-175	Os-187	Tl-205
Nd-142	Gd-162	Yb-175m	Os-188	Tl-206
Nd-143	Tb-157	Yb-176	Os-189	Pb-204
Nd-144	Tb-159	Yb-177	Os-190	Pb-205
Nd-145	Tb-160	Lu-175	Os-190m	Pb-206
Nd-146	Tb-161	Lu-176	Os-191	Pb-207
Nd-147	Tb-162	Lu-176m	Os-191m	Pb-208
Nd-148	Dy-156	Lu-177	Os-192	Pb-209
Nd-149	Dy-157	Lu-177m	Os-193	Bi-208
Nd-150	Dy-158	Hf-174	Os-194	Bi-209
Nd-151	Dy-159	Hf-175	Ir-191	Bi-210
Pm-145	Dy-160	Hf-176	Ir-192	Bi-210m
Pm-147	Dy-161	Hf-177	Ir-192m	Bi-211
Pm-148	Dy-162	Hf-178	Ir-193	Po-210
Pm-148m	Dy-163	Hf-178m	Ir-194	Po-211
Pm-149	Dy-164			Po-211m

[a]Dummy nuclide for code's internal use.

Table F7.B.2 ORIGEN-S actinides

He-4	Po-214	Th-232	Np-239	Cm-242
Tl-206	Po-215	Th-233	Np-240m	Cm-243
Tl-207	Po-216	Th-234	Np-240	Cm-244
Tl-208	Po-218	Pa-231	Np-241	Cm-245
Tl-209	At-217	Pa-232	Pu-236	Cm-246
Pb-206	Rn-218	Pa-233	Pu-237	Cm-247
Pb-207	Rn-219	Pa-234m	Pu-238	Cm-248
Pb-208	Rn-220	Pa-234	Pu-239	Cm-249
Pb-209	Rn-222	Pa-235	Pu-240	Cm-250
Pb-210	Fr-221	U-230	Pu-241	Cm-251
Pb-211	Fr-223	U-231	Pu-242	Bk-249
Pb-212	Ra-222	U-232	Pu-243	Bk-250
Pb-214	Ra-223	U-233	Pu-244	Bk-251
Bi-208	Ra-224	U-234	Pu-245	Cf-249
Bi-209	Ra-225	U-235	Pu-246	Cf-250
Bi-210m	Ra-226	U-236	Am-239	Cf-251
Bi-210	Ra-228	U-237	Am-240	Cf-252
Bi-211	Ac-225	U-238	Am-241	Cf-253
Bi-212	Ac-227	U-239	Am-242m	Cf-254
Bi-213	Ac-228	U-240	Am-242	Cf-255
Bi-214	Th-226	U-241	Am-243	Es-253
Po-210	Th-227	Np-235	Am-244m	Es-254m
Po-211m	Th-228	Np-236m	Am-244	Es-254
Po-211	Th-229	Np-236	Am-245	Es-255
Po-212	Th-230	Np-237	Am-246	S-250[a]
Po-213	Th-231	Np-238	Cm-241	

[a]Dummy nuclide for code's internal use.

Table F7.B.3 ORIGEN-S fission products

H-3	Ga-75	Cu-81	Se-86	Y-91
Li-6	Ge-75	Zn-81	Br-86	Y-91m
Li-7	Ge-75m	Ga-81	Br-86m	Zr-91
Be-9	As-75	Ge-81	Kr-86	Nb-91
Be-10	Ni-76	As-81	Rb-86	Se-92
C-14	Cu-76	Se-81	Rb-86m	Br-92
Ni-66	Zn-76	Se-81m	Sr-86	Kr-92
Cu-66	Ga-76	Br-81	Ge-87	Rb-92
Zn-66	Ge-76	Kr-81	As-87	Sr-92
Cu-67	As-76	Kr-81m	Se-87	Y-92
Zn-67	Se-76	Zn-82	Br-87	Zr-92
Zn-68	Ni-77	Ga-82	Kr-87	Nb-92
Zn-69	Cu-77	Ge-82	Rb-87	Se-93
Zn-69m	Zn-77	As-82	Sr-87	Br-93
Ga-69	Ga-77	As-82m	Sr-87m	Kr-93
Zn-70	Ge-77	Se-82	Ge-88	Rb-93
Ga-70	Ge-77m	Br-82	As-88	Sr-93
Ge-70	As-77	Br-82m	Se-88	Y-93
Zn-71	Se-77	Kr-82	Br-88	Zr-93
Zn-71m	Se-77m	Zn-83	Kr-88	Nb-93
Ga-71	Ni-78	Ga-83	Rb-88	Nb-93m
Ge-71	Cu-78	Ge-83	Sr-88	Br-94
Ge-71m	Zn-78	As-83	As-89	Kr-94
Co-72	Ga-78	Se-83	Se-89	Rb-94
Ni-72	Ge-78	Se-83m	Br-89	Sr-94
Cu-72	As-78	Br-83	Kr-89	Y-94
Zn-72	Se-78	Kr-83	Rb-89	Zr-94
Ga-72	Cu-79	Kr-83m	Sr-89	Nb-94
Ge-72	Zn-79	Ga-84	Y-89	Nb-94m
Co-73	Ga-79	Ge-84	Y-89m	Br-95
Ni-73	Ge-79	As-84	As-90	Kr-95
Cu-73	As-79	Se-84	Se-90	Rb-95
Zn-73	Se-79	Br-84	Br-90	Sr-95
Ga-73	Se-79m	Br-84m	Kr-90	Y-95
Ge-73	Br-79	Kr-84	Rb-90	Zr-95
Ge-73m	Br-79m	Ga-85	Rb-90m	Nb-95
Co-74	Kr-79	Ge-85	Sr-90	Nb-95m
Ni-74	Cu-80	As-85	Y-90	Mo-95
Cu-74	Zn-80	Se-85	Y-90m	Br-96
Zn-74	Ga-80	Se-85m	Zr-90	Kr-96
Ga-74	Ge-80	Br-85	Zr-90m	Rb-96
Ge-74	As-80	Kr-85	Se-91	Sr-96
Co-75	Se-80	Kr-85m	Br-91	Y-96
Ni-75	Br-80	Rb-85	Kr-91	Zr-96
Cu-75	Br-80m	Ge-86	Rb-91	Nb-96
Zn-75	Kr-80	As-86	Sr-91	Mo-96

Table F7.B.3 (continued)

Kr-97	Zr-102	Y-107	Ru-111	In-115
Rb-97	Nb-102	Zr-107	Rh-111	In-115m
Sr-97	Mo-102	Nb-107	Pd-111	Sn-115
Y-97	Tc-102	Mo-107	Pd-111m	Tc-116
Zr-97	Tc-102m	Tc-107	Ag-111	Ru-116
Nb-97	Ru-102	Ru-107	Ag-111m	Rh-116
Nb-97m	Rh-102	Rh-107	Cd-111	Pd-116
Mo-97	Pd-102	Pd-107	Cd-111m	Ag-116
Kr-98	Sr-103	Pd-107m	Nb-112	Ag-116m
Rb-98	Y-103	Ag-107	Mo-112	Cd-116
Sr-98	Zr-103	Zr-108	Tc-112	In-116
Y-98	Nb-103	Nb-108	Ru-112	In-116m
Zr-98	Mo-103	Mo-108	Rh-112	Sn-116
Nb-98	Tc-103	Tc-108	Pd-112	Tc-117
Nb-98m	Ru-103	Ru-108	Ag-112	Ru-117
Mo-98	Rh-103	Rh-108	Cd-112	Rh-117
Tc-98	Rh-103m	Rh-108m	Mo-113	Pd-117
Rb-99	Sr-104	Pd-108	Tc-113	Ag-117
Sr-99	Y-104	Ag-108	Ru-113	Ag-117m
Y-99	Zr-104	Ag-108m	Rh-113	Cd-117
Zr-99	Nb-104	Cd-108	Pd-113	Cd-117m
Nb-99	Mo-104	Zr-109	Ag-113	In-117
Nb-99m	Tc-104	Nb-109	Ag-113m	In-117m
Mo-99	Ru-104	Mo-109	Cd-113	Sn-117
Tc-99	Rh-104	Tc-109	Cd-113m	Sn-117m
Tc-99m	Rh-104m	Ru-109	In-113	Tc-118
Ru-99	Pd-104	Rh-109	In-113m	Ru-118
Rb-100	Y-105	Rh-109m	Mo-114	Rh-118
Sr-100	Zr-105	Pd-109	Tc-114	Pd-118
Y-100	Nb-105	Pd-109m	Ru-114	Ag-118
Zr-100	Mo-105	Ag-109	Rh-114	Ag-118m
Nb-100	Tc-105	Ag-109m	Pd-114	Cd-118
Nb-100m	Ru-105	Cd-109	Ag-114	In-118
Mo-100	Rh-105	Nb-110	Cd-114	In-118m
Tc-100	Rh-105m	Mo-110	In-114	Sn-118
Ru-100	Pd-105	Tc-110	In-114m	Ru-119
Rb-101	Y-106	Ru-110	Sn-114	Rh-119
Sr-101	Zr-106	Rh-110	Mo-115	Pd-119
Y-101	Nb-106	Rh-110m	Tc-115	Ag-119
Zr-101	Mo-106	Pd-110	Ru-115	Cd-119
Nb-101	Tc-106	Ag-110	Rh-115	Cd-119m
Mo-101	Ru-106	Ag-110m	Pd-115	In-119
Tc-101	Rh-106	Cd-110	Ag-115	In-119m
Ru-101	Rh-106m	Nb-111	Ag-115m	Sn-119
Sr-102	Pd-106	Mo-111	Cd-115	Sn-119m
Y-102	Ag-106	Tc-111	Cd-115m	Ru-120

Table F7.B.3 (continued)

Rh-120	Pd-125	Te-129m	Sb-134	Te-139
Pd-120	Ag-125	I-129	Sb-134m	I-139
Ag-120	Cd-125	Xe-129	Te-134	Xe-139
Cd-120	In-125	Xe-129m	I-134	Cs-139
In-120	In-125m	Cd-130	I-134m	Ba-139
In-120m	Sn-125	In-130	Xe-134	La-139
Sn-120	Sn-125m	Sn-130	Xe-134m	Ce-139
Rh-121	Sb-125	Sb-130	Cs-134	Pr-139
Pd-121	Te-125	Sb-130m	Cs-134m	Te-140
Ag-121	Te-125m	Te-130	Ba-134	I-140
Cd-121	Pd-126	I-130	Sn-135	Xe-140
In-121	Ag-126	I-130m	Sb-135	Cs-140
In-121m	Cd-126	Xe-130	Te-135	Ba-140
Sn-121	In-126	Cd-131	I-135	La-140
Sn-121m	Sn-126	In-131	Xe-135	Ce-140
Sb-121	Sb-126	Sn-131	Xe-135m	Pr-140
Rh-122	Sb-126m	Sb-131	Cs-135	Te-141
Pd-122	Te-126	Te-131	Cs-135m	I-141
Ag-122	Xe-126	Te-131m	Ba-135	Xe-141
Cd-122	Ag-127	I-131	Ba-135m	Cs-141
In-122	Cd-127	Xe-131	Sn-136	Ba-141
In-122m	In-127	Xe-131m	Sb-136	La-141
Sn-122	In-127m	Cd-132	Te-136	Ce-141
Sb-122	Sn-127	In-132	I-136	Pr-141
Sb-122m	Sn-127m	Sn-132	I-136m	Nd-141
Te-122	Sb-127	Sb-132	Xe-136	Te-142
Rh-123	Te-127	Sb-132m	Cs-136	I-142
Pd-123	Te-127m	Te-132	Ba-136	Xe-142
Ag-123	I-127	I-132	Ba-136m	Cs-142
Cd-123	Xe-127	Xe-132	Sb-137	Ba-142
In-123	Ag-128	Cs-132	Te-137	La-142
In-123m	Cd-128	Ba-132	I-137	Ce-142
Sn-123	In-128	In-133	Xe-137	Pr-142
Sn-123m	Sn-128	Sn-133	Cs-137	Pr-142m
Sb-123	Sb-128	Sb-133	Ba-137	Nd-142
Te-123	Sb-128m	Te-133	Ba-137m	I-143
Te-123m	Te-128	Te-133m	Sb-138	Xe-143
Pd-124	I-128	I-133	Te-138	Cs-143
Ag-124	Xe-128	I-133m	I-138	Ba-143
Cd-124	Cd-129	Xe-133	Xe-138	La-143
In-124	In-129	Xe-133m	Cs-138	Ce-143
Sn-124	Sn-129	Cs-133	Cs-138m	Pr-143
Sb-124	Sn-129m	Ba-133	Ba-138	Nd-143
Sb-124m	Sb-129	In-134	La-138	I-144
Te-124	Te-129	Sn-134	Sb-139	Xe-144

Table F7.B.3 (continued)

Cs-144	Ba-149	Ce-154	Pm-160	Yb-168
Ba-144	La-149	Pr-154	Sm-160	Er-169
La-144	Ce-149	Nd-154	Eu-160	Tm-169
Ce-144	Pr-149	Pm-154	Gd-160	Yb-169
Pr-144	Nd-149	Pm-154m	Tb-160	Er-170
Pr-144m	Pm-149	Sm-154	Dy-160	Tm-170
Nd-144	Sm-149	Eu-154	Nd-161	Tm-170m
I-145	Eu-149	Gd-154	Pm-161	Yb-170
Xe-145	Cs-150	La-155	Sm-161	Er-171
Cs-145	Ba-150	Ce-155	Eu-161	Tm-171
Ba-145	La-150	Pr-155	Gd-161	Yb-171
La-145	Ce-150	Nd-155	Tb-161	Er-172
Ce-145	Pr-150	Pm-155	Dy-161	Tm-172
Pr-145	Nd-150	Sm-155	Pm-162	Yb-172
Nd-145	Pm-150	Eu-155	Sm-162	
Pm-145	Sm-150	Gd-155m[a]	Eu-162	
Sm-145	Eu-150	Gd-155	Gd-162	
Xe-146	Ba-151	Ce-156	Tb-162	
Cs-146	La-151	Pr-156	Tb-162m	
Ba-146	Ce-151	Nd-156	Dy-162	
La-146	Pr-151	Pm-156	Sm-163	
Ce-146	Nd-151	Sm-156	Eu-163	
Pr-146	Pm-151	Eu-156	Gd-163	
Nd-146	Sm-151	Gd-156	Tb-163	
Pm-146	Eu-151	Ce-157	Tb-163m	
Sm-146	Ba-152	Pr-157	Dy-163	
Xe-147	La-152	Nd-157	Sm-164	
Cs-147	Ce-152	Pm-157	Eu-164	
Ba-147	Pr-152	Sm-157	Gd-164	
La-147	Nd-152	Eu-157	Tb-164	
Ce-147	Pm-152	Gd-157	Dy-164	
Pr-147	Pm-152m	Pr-158	Sm-165	
Nd-147	Sm-152	Nd-158	Eu-165	
Pm-147	Eu-152	Pm-158	Gd-165	
Sm-147	Eu-152m	Sm-158	Tb-165	
Cs-148	Gd-152	Eu-158	Dy-165	
Ba-148	La-153	Gd-158	Dy-165m	
La-148	Ce-153	Pr-159	Ho-165	
Ce-148	Pr-153	Nd-159	Dy-166	
Pr-148	Nd-153	Pm-159	Ho-166	
Nd-148	Pm-153	Sm-159	Ho-166m	
Pm-148	Sm-153	Eu-159	Er-166	
Pm-148m	Eu-153	Gd-159	Er-167	
Sm-148	Gd-153	Tb-159	Er-167m	
Cs-149	La-154	Nd-160	Er-168	

[a]Dummy nuclide for code's internal use.

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Computing Applications Division

ICE: MODULE TO MIX MULTIGROUP CROSS SECTIONS

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ABSTRACT

ICE is a cross-section mixing code that will accept cross sections from an AMPX working library and produce mixed cross sections in the AMPX working library format, ANISN format, the group-independent ANISN format, and the Monte Carlo processed cross-section library format. User input is in the free-form or fixed-form FIDO structure. The code is also operable as a module in the AMPX system.

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F8.1 INTRODUCTION

ICE (Intermixed Cross Sections Effortlessly) is a cross-section mixing code that will accept cross sections from an AMPX[1] working library and produce mixed cross sections in four formats: (1) AMPX working library format, (2) ANISN[2] format, (3) group-independent ANISN format, and (4) the Monte Carlo processed cross-section library format. User input is in the free-form or fixed-form FIDO structure, described in Sect. M10 of this manual.

The code was developed to allow efficient mixing with minimum user effort and with reduced core storage requirements. The code is also operable as a module in the AMPX system. The SCALE version of ICE is the latest in a series[3,4] of versions of the program.

In SCALE, ICE is used exclusively to prepare mixed cross-section libraries for use in Monte Carlo programs; in SAS3, it produces a library for MORSE-SGC, and in CSASI and CSASIX it produces a library for KENO-V.a.

F8.1.1 AMPX WORKING LIBRARY FORMAT

The AMPX working library format is described in detail in Sect. F2.3.8 of this report. As noted earlier, ICE will accept input only in this format, and one of its options is to output data in this format.

F8.1.2 STANDARD ANISN FORMAT

In the second output option, cross sections are written in ANISN binary format on logical IOT2 or will be output on punched cards on logical 7. In both cases, "blocks" of cross sections are specified using two types of "records." A "block" of data in the ANISN context consists of values for one P_ℓ matrix of the cross sections of a nuclide or a mixture. The first "record" or card for a block contains 16 words as follows:

1. NOG - the number of energy groups in the block.
2. IHM - the table length of the cross sections in the block.
3. ICT - a control word which is 0 normally and is 7 for the last record in the cross-section set.
4. ID - a numeric identifier for the cross-section block.

5-16. (Text(i), i = 1,12) - 48 characters of text to describe the cross-section block.

In the case of the card-image format, the above is written:

(1H',2I6,I4,I6,12A4)

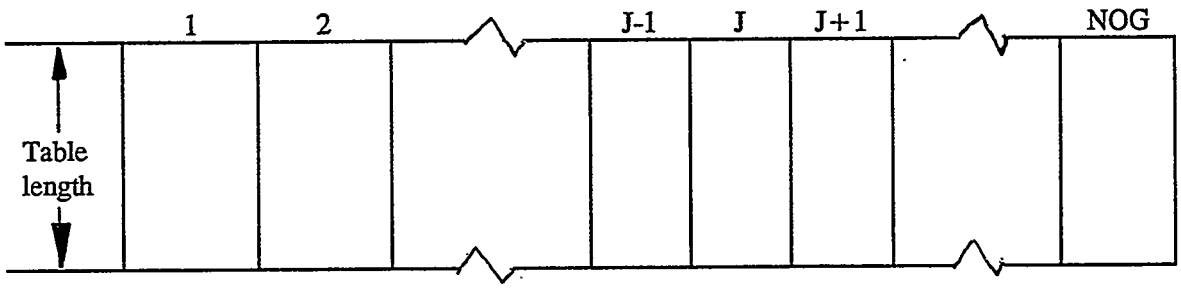
The cross sections in a block are in a rectangular array and are written:

((XS(I,J), I=1, IHM), J=1, NOG)

In the case of card output, the values are written using the free-form FIDO schemes discussed in Sect. M10.

A schematic of the structure is shown below:

GROUP NUMBER



Within a column for a group, the group-averaged values for various processes, along with the values for scattering to the group G, are given:

Position	Type of Value
1	(user specified)
.	
.	
.	
.	
IHT-4	χ
IHT-3	Σ_f
IHT-2	Σ_a
IHT-1	$\overline{\nu\Sigma_f}$
IHT	Σ_t
.	.
.	.
.	.
IHS-2	$\Sigma(G+2\rightarrow G)$
IHS-1	$\Sigma(G+1\rightarrow G)$
IHS	$\Sigma(G\rightarrow G)$
IHS+1	$\Sigma(G-1\rightarrow G)$
.	.
.	.
.	.
.	.
IHM	

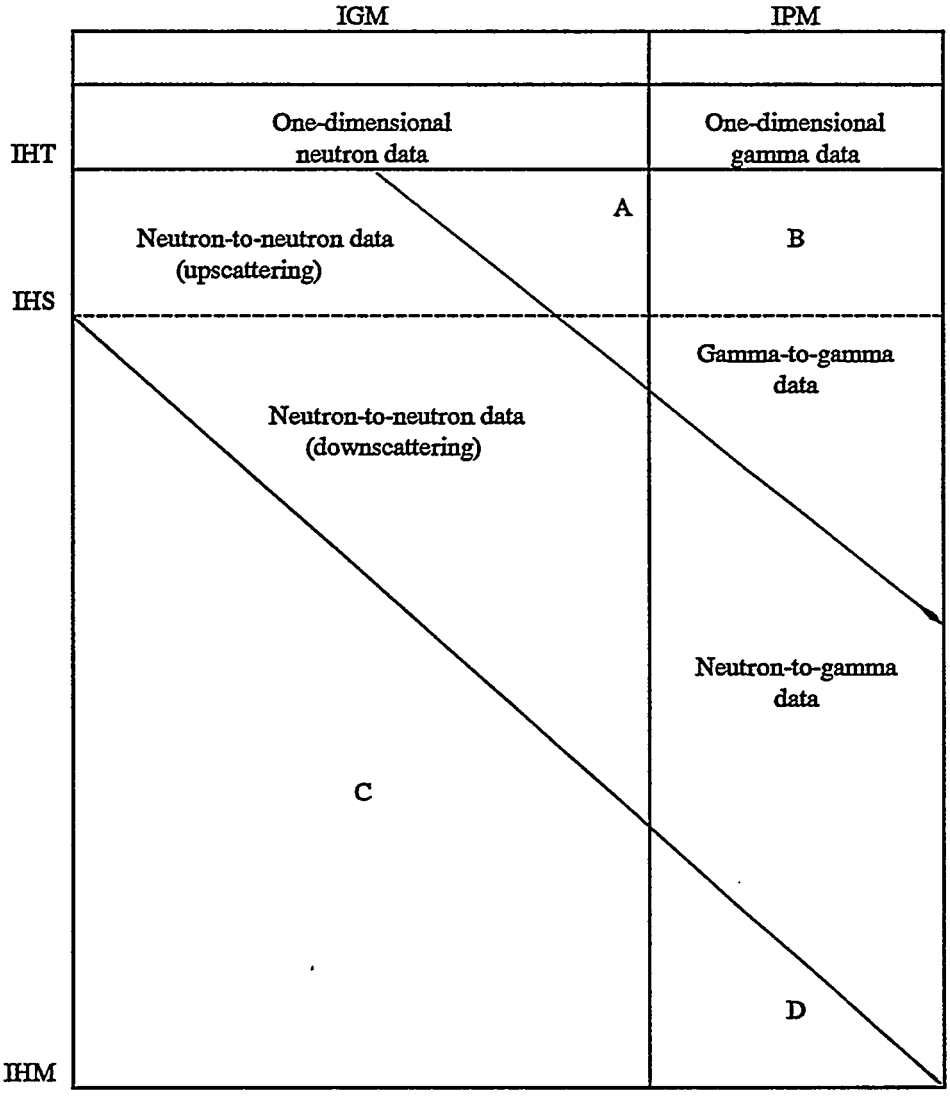
where IHT is the position of the total cross-section values in the table, IHS is the within-group scattering position, and IHM is the table length. Note that positions that are undefined do not exist. For example, when IHT = 3, there are no values for Σ_f in the table, etc., or if IHT = 3 and IHS = 4, there are no upscatters in the table. When IHM is less than (IHS + total number of groups less one), some possible downscatters are truncated, etc.

Another characteristic to note concerning ANISN values is that the matrices are multiplied by $(2\ell+1)$; i.e., P_0 terms are multiplied by unity, P_1 terms by three, etc.

In some analyses, especially for certain shielding problems, calculations are made with ANISN cross sections which contain both neutron and gamma cross-section information. These libraries contain three kinds of scattering data:

1. neutron-to-neutron,
2. neutron-to-gamma, and
3. gamma-to-gamma.

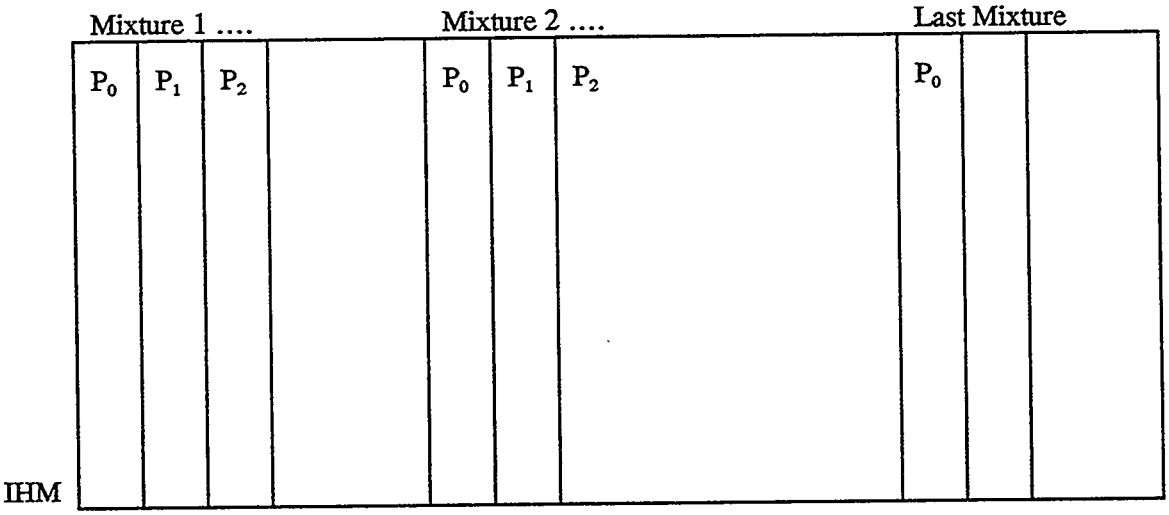
For the forward (as opposed to adjoint) case, the cross sections will be arranged as in the following diagram:



where IGM and IPM are the number of neutron and gamma groups, respectively, areas C and D are zero because they represent transfers from nonexistent groups, A is zero because gammas do not generally transfer to neutron groups, and B is zero because gammas do not upscatter.

F8.1.3 GROUP-INDEPENDENT ANISN FORMAT

By option, cross sections can be output on logical unit IOT3 in a special binary format called the group-independent form. This form amounts to a rearrangement of the structure discussed in the previous section to where the group index is on the outside. In this case, the ordering is still by columns of length IHM. No header records are included and the group-independent file will contain one record per group:



In this arrangement, the user must know the number of groups, the table length, etc., the number of mixtures and the order of scattering for each mixture, as these will have to be specified to the code that uses the data.

F8.1.4 MONTE CARLO LIBRARY FORMAT

By option, a special Monte Carlo library is written in binary format on logical IOT4. This library can be directly input to MORSE-SGC (Sect. F9) and/or to KENO-V (Sect. F11), thereby allowing these modules to bypass cross-section mixing.

In describing the structure of the library, it will be necessary to speak in terms of forward versus adjoint applications and of primary versus secondary particle data types. One must also concern himself with so-called fully coupled libraries versus those libraries that are not fully coupled.

The structure of the Monte Carlo library is shown below:

	Record Type
Header Record	1
Primary Group Structure	2
Secondary Group Structure (if applicable)	2
The following record pattern is repeated for all mixtures on the library.	
Mixture Identification	3
Primary One-Dimensional Data	4
Secondary One-Dimensional Data (if applicable)	4
Pointer Array for Primary-to-Primary and Secondary-to-Secondary	5
Pointer Array for Primary-to-Secondary (if applicable)	5
Primary-to-Primary Scattering Data	
Secondary-to-Secondary Scattering Data (if applicable)	
Primary-to-Secondary Scattering Data (if applicable)	

The internal structure of the three blocks of scattering data of order NL and NSCT angles is shown below:

	Record Type
Probabilities for Group-to-Group Scattering	6
f_1 Legendre Coefficients for Group-to-Group Scattering	6
. . .	
f_{NL} Legendre Coefficients for Group-to-Group Scattering	6
When NSCT > 0, there will be 2*NSCT records following:	
Probabilities for Group/Angle 1 Matrices	7
Cosines for Group/Angle 1 Matrices	8
Probabilities for Group/Angle 2 Matrices	7
. . .	
Cosines for Group/Angle NSCT Matrices	8

Without going into a development of adjoint forms of multigroup equations, suffice it to say that the adjoint equations for a particular group involve source terms that, instead of using scattering terms from other groups to that group, use terms from the group to other groups. This inversion of terms makes it convenient to reverse the order of iteration through energy groups from a high-to-low energy ordering to a low-to-high ordering. In many programs that solve adjoint and forward problems, the approach has been to invert cross-section blocks appropriately such that the same indexing and coding solves both cases, rather than to build dual logic into the coding. In this case, the first group becomes the last group and transfer matrices are rearranged, etc.

In the case of a neutron/gamma coupled forward solution where the solution scans from the first (highest-energy) neutron group to the last gamma group, it is natural to think of the neutrons as primary particles and the gammas as secondary particles. If we adopt this convention, then the matrix inversion required to do the adjoint case will locate the gammas in the "primary" position and the neutrons become "secondary."

Two types of coupled neutron/gamma AMPX working libraries can be treated by ICE—a so-called fully coupled library and a library that is not fully coupled. In the fully coupled case, the transfer matrices for neutron-to-neutron, neutron-to-gamma, and gamma-to-gamma are all combined in a single matrix in much the same structure as shown in the discussion of ANISN formatted data; whereas, in the other case, these three blocks of data are carried separately.

Eight types of data or records may be used in creating the Monte Carlo library:

Type	Kind of Information
1	Header Information
2	Group Structure
3	Mixture or Nuclide Identifier
4	One-Dimensional Data
5	Transfer Matrix Pointers
6	Group-to-Group Scattering Probabilities
7	Probabilities for Group/Angle Matrices
8	Cosines for Group/Angle Matrices

Record Type 1 (Header Information)

The first record on the Monte Carlo library is the header record, and it serves to define the number of mixtures on the library, the number of primary and secondary groups, etc. It has 50 words:

Word	Type of Information
1	IDTAPE - Tape identification number
2	NMIX - Number of mixtures on library
3	NPRIM - Number of "primary" groups
4	NSEC - Number of "secondary" groups
5	ICP - 0, not fully coupled 1, fully coupled
6	IADJT - 0, forward library 1, adjoint library
7	IFTG - first thermal group (i.e., with upscatter to it) in the primary groups
8	JFTG - last thermal group in the primary groups
9	KFTG - first group in the primary groups with transfers to secondary groups
10	LFTG - last group in the primary groups with transfers to secondary groups
11	NSCT - maximum number of scattering angles used in group-to-group/angle probability scattering data for a mixture on the library
12	NNGA - number of input primary groups (bottom groups can be truncated from NPRIM)
13	NGGA - number of input secondary groups
14	NOPT - truncation option (This option applies for NNGA and NGGA.) 0, downscatters to truncated groups kept 1, downscatters to truncated groups are summed into last downscatter cross section for a group 2, downscatters to missing groups are dropped and no adjustments are made
15-50	The remainder of the record is filled with zeroes.

Record Type 2 (Group Structure)

This record specifies an energy group structure followed by the corresponding lethargy structure with the "lethargy zero" taken at 107 eV. The energies are in descending order. If the number of groups plus one is IGP, the structure is

$$(E(I),I=1,IGP),\ (U(I),I=1,IGP)\ ,$$

where E and U are arrays for energies and lethargies, respectively.

Record Type 3 (Nuclide or Mixture Identifier)

This record consists of 50 words and defines the lengths and types of records that are needed to represent the cross sections for a mixture. The makeup is the following:

Word(s)	Contents
1-18	Textual information (72 characters) describing the mixture
19	An integer identifier for the mixture
20	Zero
21	Length of primary-to-secondary scattering probability arrays (not fully coupled case)
22	Length of secondary-to-secondary scattering probability arrays (not fully coupled case)
23	Length of primary-to-primary scattering probability arrays (in the fully coupled case this is the length of the fully coupled matrices)
24	Order of scattering for the mixture
25	Number of scattering angles for the mixture
26	0, scattering data are fully coupled 1, scattering data are not fully coupled
27	Zero
28	Number of one-dimensional (1-D) (group averaged) processes in the primary data
29-40	Zero
41	Number of 1-D processes in the secondary data
42-49	Zero
50	Number of records required to store data for the mixture (should include the identifier record).

Record Type 4 (1-D Data)

In describing cross sections for SCALE, the term "1-D" designates group-averaged data given as a function of process and energy group, as opposed to two-dimensional cross sections, which refer to transfer matrices. The various processes in the 1-D record are identified by integers that typically correspond to the ENDF/B[5] MT-numbers that identify processes. For example, MT = 1 is used to identify total values, MT = 2 for elastic scattering, etc.

ICE also constructs cross sections for up to six extra processes as follows:

New Primary 1-D Data

MT	Description
2002	Sum of the transfer cross sections out of a group (truncated groups are not included in the sum)
2100	Sum of the terms left out of MT = 2002 due to a truncation of groups
2102	Sum of the primary-to-secondary transfers (for the not fully coupled case only)

New Secondary 1-D Data

MT	Description
2502	Equivalent to 2002 but for secondaries
2600	Equivalent to 2100
2602	Equivalent to 2102 but only for the adjoint case

The 1-D arrays are a combination of integer and floating point data arranged as follows:

MT for first process
Σ for group 1 of first process
.
.
.
.
Σ for last group of first process
MT for second process
for group 1 of second process
.
.
.
.
Σ for last group of last process

Record Type 5 (Transfer Matrix Pointers)

As the number of energy groups increases, the number of possible group-to-group transfers increases by the square of the number of groups. Clearly, one can quickly reach a point where it is inconvenient to store complete transfer matrices, unless special means are provided to eliminate impossible and/or nonexistent terms from these matrices. The number of terms needed can vary dramatically from nuclide to nuclide for many large group structures.

Because of these characteristics, the Monte Carlo library structure contains only those terms that span the total range of scatter for a group. This step is accomplished by specifying the transfer matrix with both the pointer array being discussed here and the actual transfer array.

The pointer array is dimensioned by three times the number of source groups for the block of data the pointers are associated with. These three words for a group are

1. a pointer to the word in the transfer array at which the cross sections for scattering from this group begin,

2. a pointer to the word in the transfer array at which the cross sections for scattering from this group end, and

3. the sink group corresponding to the first transfer term out of the group.

This arrangement assumes that the sink groups increase in number in the string of terms for a group. For example, if the triplet for group 5 was (53, 57, 5), then the cross sections in the transfer matrix would be:

Location	Value
53	$\Sigma(5\rightarrow5)$
54	$\Sigma(5\rightarrow6)$
55	$\Sigma(5\rightarrow7)$
56	$\Sigma(5\rightarrow8)$
57	$\Sigma(5\rightarrow9)$

The list structure of the pointer array is

((IPT(J,I),J=1,3), I=1,NGROUPS)

Record Type 6 (Group-to-Group Scattering Probabilities)

This record type is used to present a group-to-group transfer matrix. The units are probabilities in the case of the P_0 matrix and are the coefficients of a Legendre fit to the transfer for $\ell > 0$. Note that in the latter case, they are coefficients and are normalized such that $f_0 = 1.0$. They do not contain a $(2\ell + 1)$ factor as in the case of the ANISN formats discussed previously. The terms in the P_ℓ arrays are in a one-to-one correspondence with the P_0 array. The pointer array described above defines the terms in the matrix.

The list structure is

(XS(I), I=1, LENGTH)

where LENGTH is the 21st, 22nd, or 23rd word in the mixture identification record.

Record Type 7 (Probability for Group/Angle Matrices)

The structure of this record is the same as Record Type 6. There will be one of these records for each of the scattering angles specified for the nuclide.

Record Type 8 (Cosines for Group/Angle Matrices)

The structure of this record is as for Record Type 6. These values are the cosines of the angles corresponding to the probabilities presented in Record Type 7.

The techniques for choosing the probabilities and angles are discussed in Sect. F9.D.2.

F8.2 THEORY

Most of the "theory" for ICE operations is based on simple algebra. Some operations require the use of simple approximations as presented below.

F8.2.1 CROSS-SECTION MIXING FOR AMPX AND ANISN LIBRARIES

For the options that produce AMPX working or ANISN libraries, the mixing of cross sections involves a very simple summing of constituent values times a number density for the constituent, that is, Σ, a macroscopic value, is determined by

$$\Sigma = \sum_j N_j \sigma_j ,$$

where the j are the individual nuclides in the mixture whose number density and microscopic cross sections are N_j and σ_j, respectively.

The only exceptions to the above rule are for fissionable mixtures where the number of neutrons per fission, υ_g, or a fission spectrum, χ_g, is required:

$$\nu_g = \frac{\sum_j N_j \nu_{gj} \sigma_{gj}}{\sum_j N_j \sigma_{fgj}} .$$

This χ_g is defined as the fraction of the fission neutrons produced by the mixture which fall in group g. By definition,

$$\sum_g \chi_g = 1.0 .$$

ICE uses the following scheme to determine χ. First, terms F_g are determined by

$$F_g = \sum_j N_j \chi_{gj} \sum_{g'} \overline{\nu\sigma}_{fg',j} \hat{\phi}_{g'} , \qquad \text{(F8.2.1)}$$

where $\overline{\nu\sigma}_{fg,j}$ is the average of the product of υ times σ_f for the nuclide, $\chi_{g,j}$ is the nuclide fission spectrum, and $\hat{\phi}_g$ is an estimate for the integrated flux in group g'. Once the F_g are determined, χ_g is determined by normalizing the sum of F_g to unity. In the above expression, the unknown parameter is the flux and ICE makes five options available for its determination. These options are specified as the seventh parameter (KOPT) in the 1$ array of the input. (See Sect. F8.4.)

Option 1 (KOPT = O)

In this case, χ is taken to be that of the nuclide that has the largest value for

$$N_j \sum_g \overline{\nu\sigma}_{fg} \phi_g ,$$

where ϕ_g is arbitrarily set to 1.0 for all groups. This option obviously involves a great deal of approximation for the flux.

Option 2 (KOPT = 1)

In this case, values for group fluxes are determined by some external means and used in expression (F8.2.1).

Option 3 (KOPT = 2)

In this case, Eq. (F8.2.1) is used with the following set of expressions taken to approximate a typical thermal reactor spectrum.

(1) $\phi(E) = C_2 E e^{-E/kT}$ $(0 < E \leq E_m)$

(2) $\phi(E) = 1.0/E$ $(E_m < E \leq E_f)$

(3) $\phi(E) = C_1 \sqrt{E}\, e^{-E/\theta}$ $(E_f < E)$.

In these expressions E_m is the upper energy cutoff for a region using a Maxwellian spectrum, E_f is the lower energy cutoff for a region using a fission spectrum, kT is the effective temperature of the medium, and θ is the temperature of the fission spectrum. All fitting parameters can be supplied as input data, or default values can be used. The normalization coefficients are selected to make the end spectra join to a 1/E spectrum interior to E_m and E_f:

$$C_1 = E_f^{-3/2} e^{E_f/\theta}$$

$$C_2 = E_m^{-2} e^{E_m/kT} .$$

In order to evaluate

$$\hat{\phi}_g \equiv \int_g dE\, \phi(E) ,$$

an equal lethargy mesh is taken within a group g such that the ratio of adjacent points is given by 0.95, that is,

$$\frac{E_{i+1}}{E_i} = 0.95 ,$$

where the E_i's are energies in the mesh and E_i descends. The mesh is adjusted when E_i, E_{i+1} spans a group boundary.

For the mesh intervals, the integral I_i is determined by evaluating the fluxes at E_i and E_{i+1} and assuming the logarithm of the flux is linear in lethargy.

Option 4 (KOPT = 3)

In this case a spectrum representative of many fast reactors was determined in an external calculation using a 119-group energy structure. This calculation was a mock-up of the ZPR-3-56B benchmark[6] and the group structure and group-integrated flux values are shown in Table F8.2.1.

The procedure for generating group fluxes is the same as for Option 3 above except that the ratio between the points in the integration mesh is taken to be 0.9. To evaluate the point fluxes in per unit energy units, the integrated fluxes are divided by the group's energy width and the value is assumed to be given at the lethargy midpoint of the group, that is,

$$\bar{E}_g = \sqrt{E_g^L E_g^H},$$

where E_g^L, E_g^H, $\bar{E}_g$ are the lower limit, the upper limit, and the "average" energy of the group, respectively. To evaluate fluxes at a point, these "average" fluxes are assumed to vary log-log in energy, as for Option 3.

Option 5 (KOPT = 4)

In many AMPX libraries, the integrals of the spectrum used to determine the multigroup values are carried on the library for each nuclide. With KOPT = 4, ICE will use this nuclide-dependent spectrum to determine χ_g. This option should be exercised with caution, however, for no attempt is made to ensure that the individual spectra are consistently normalized.

F8.2.2 CROSS-SECTION MIXING FOR THE MONTE CARLO LIBRARY

In order to mix cross sections for the Monte Carlo library, exactly the same schemes are used as for the ANISN or AMPX options. However, because of the special techniques employed in Monte Carlo programs, the units for the data are expressed in probabilities, instead of cross sections.

In the case of the P_0 group-to-group probabilities, Record Type 6 in Sect. F8.1.4, the data are in probability units, such that

$$\sum_j P_0(i \to j) = 1.0$$

for the terms given, whether or not terms have been truncated from the transfer matrix, that is, the probabilities are normalized to the MT = 2002 or 2502 1-D values.

Table F8.2.1 Flux values from a ZPPR-3 calculation

Group	Limits	Flux	Average energy	Flux per unit energy
1	1.22E+07-1.49E+07	9.31E-03	1.35E+07	3.44E-09
2	1.00E+07-1.22E+07	3.67E-02	1.11E+07	1.66E-08
3	8.19E+06-1.00E+07	1.09E-01	9.05E+06	6.01E-08
4	6.70E+06-8.19E+06	2.55E-01	7.41E+06	1.72E-07
5	5.49E+06-6.70E+06	4.95E-01	6.07E+06	4.07E-07
6	4.49E+06-5.49E+06	8.29E-01	4.97E+06	8.33E-07
7	3.68E+06-4.49E+06	1.13E+00	4.07E+06	1.39E-06
8	3.17E+06-3.68E+06	1.09E+00	3.41E+06	2.13E-06
9	3.01E+06-3.17E+06	5.08E-01	3.09E+06	3.29E-06
10	2.87E+06-3.01E+06	5.26E-01	2.94E+06	3.58E-06
11	2.73E+06-2.87E+06	5.63E-01	2.79E+06	4.03E-06
12	2.59E+06-2.73E+06	6.44E-01	2.66E+06	4.85E-06
13	2.47E+06-2.59E+06	6.42E-01	2.53E+06	5.08E-06
14	2.39E+06-2.47E+06	4.57E-01	2.43E+06	5.66E-06
15	2.37E+06-2.39E+06	1.40E-01	2.38E+06	7.04E-06
16	2.31E+06-2.37E+06	4.04E-01	2.34E+06	6.92E-06
17	2.23E+06-2.31E+06	4.90E-01	2.27E+06	6.48E-06
18	2.12E+06-2.23E+06	6.64E-01	2.18E+06	6.10E-06
19	2.02E+06-2.12E+06	6.30E-01	2.07E+06	6.08E-06
20	1.92E+06-2.02E+06	6.57E-01	1.97E+06	6.68E-06
21	1.83E+06-1.92E+06	6.98E-01	1.87E+06	7.45E-06
22	1.74E+06-1.83E+06	7.91E-01	1.78E+06	8.88E-06
23	1.65E+06-1.74E+06	8.07E-01	1.69E+06	9.53E-06
24	1.57E+06-1.65E+06	7.56E-01	1.61E+06	9.38E-06
25	1.50E+06-1.57E+06	8.35E-01	1.53E+06	1.09E-05
26	1.42E+06-1.50E+06	8.86E-01	1.46E+06	1.21E-05
27	1.35E+06-1.42E+06	9.19E-01	1.39E+06	1.33E-05
28	1.29E+06-1.35E+06	7.48E-01	1.32E+06	1.13E-05
29	1.22E+06-1.29E+06	9.49E-01	1.26E+06	1.51E-05
30	1.16E+06-1.22E+06	1.08E+00	1.19E+06	1.81E-05
31	1.11E+06-1.16E+06	9.90E-01	1.14E+06	1.74E-05
32	1.00E+06-1.11E+06	1.52E+00	1.05E+06	1.44E-05
33	9.62E+05-1.00E+06	6.04E-01	9.82E+05	1.47E-05
34	9.07E+05-9.62E+05	1.03E+00	9.34E+05	1.89E-05
35	8.63E+05-9.07E+05	1.02E+00	8.85E+05	2.31E-05
36	8.21E+05-8.63E+05	1.31E+00	8.42E+05	3.11E-05
37	7.81E+05-8.21E+05	1.33E+00	8.01E+05	3.32E-05
38	7.43E+05-7.81E+05	1.45E+00	7.62E+05	3.81E-05
39	7.07E+05-7.43E+05	1.39E+00	7.24E+05	3.84E-05
40	6.72E+05-7.07E+05	1.44E+00	6.89E+05	4.18E-05
41	6.39E+05-6.72E+05	1.65E+00	6.55E+05	5.03E-05

Table F8.2.1 (continued)

Group	Limits	Flux	Average energy	Flux per unit energy
42	6.08E+05-6.39E+05	1.79E+00	6.23E+05	5.74E-05
43	5.78E+05-6.08E+05	1.84E+00	5.93E+05	6.20E-05
44	5.50E+05-5.78E+05	1.91E+00	5.64E+05	6.77E-05
45	5.23E+05-5.50E+05	2.09E+00	5.37E+05	7.79E-05
46	4.98E+05-5.23E+05	2.18E+00	5.10E+05	8.54E-05
47	4.50E+05-4.98E+05	3.16E+00	4.74E+05	6.67E-05
48	4.08E+05-4.50E+05	2.35E+00	4.29E+05	5.48E-05
49	3.69E+05-4.08E+05	2.77E+00	3.88E+05	7.14E-05
50	3.34E+05-3.69E+05	3.77E+00	3.51E+05	1.07E-04
51	3.02E+05-3.34E+05	4.14E+00	3.17E+05	1.30E-04
52	2.99E+05-3.02E+05	4.34E-01	3.00E+05	1.25E-04
53	2.97E+05-2.99E+05	1.79E-01	2.98E+05	1.38E-04
54	2.95E+05-2.97E+05	4.23E-01	2.96E+05	1.58E-04
55	2.87E+05-2.95E+05	1.08E+00	2.91E+05	1.49E-04
56	2.73E+05-2.87E+05	2.01E+00	2.80E+05	1.43E-04
57	2.47E+05-2.73E+05	4.27E+00	2.60E+05	1.64E-04
58	2.24E+05-2.47E+05	4.21E+00	2.35E+05	1.79E-04
59	2.13E+05-2.24E+05	2.04E+00	2.18E+05	1.87E-04
60	2.02E+05-2.13E+05	1.91E+00	2.08E+05	1.84E-04
61	1.93E+05-2.02E+05	2.01E+00	1.97E+05	2.04E-04
62	1.83E+05-1.93E+05	2.18E+00	1.88E+05	2.32E-04
63	1.74E+05-1.83E+05	2.60E+00	1.79E+05	2.91E-04
64	1.66E+05-1.74E+05	2.07E+00	1.70E+05	2.44E-04
65	1.58E+05-1.66E+05	2.26E+00	1.62E+05	2.79E-04
66	1.50E+05-1.58E+05	2.11E+00	1.54E+05	2.75E-04
67	1.43E+05-1.50E+05	1.79E+00	1.46E+05	2.45E-04
68	1.36E+05-1.43E+05	2.19E+00	1.39E+05	3.15E-04
69	1.29E+05-1.36E+05	2.28E+00	1.32E+05	3.44E-04
70	1.23E+05-1.29E+05	2.34E+00	1.26E+05	3.71E-04
71	1.17E+05-1.23E+05	2.25E+00	1.20E+05	3.76E-04
72	1.11E+05-1.17E+05	2.14E+00	1.14E+05	3.75E-04
73	9.80E+04-1.11E+05	5.14E+00	1.04E+05	3.94E-04
74	8.65E+04-9.80E+04	5.16E+00	9.21E+04	4.48E-04
75	8.25E+04-8.65E+04	1.38E+00	8.45E+04	3.44E-04
76	7.95E+04-8.25E+04	2.02E+00	8.10E+04	6.73E-04
77	7.20E+04-7.95E+04	3.62E+00	7.57E+04	4.83E-04
78	6.74E+04-7.20E+04	3.07E+00	6.97E+04	6.64E-04
79	5.66E+04-6.74E+04	7.04E+00	6.17E+04	6.51E-04
80	5.25E+04-5.66E+04	1.58E+00	5.45E+04	3.87E-04
81	4.63E+04-5.25E+04	4.54E+00	4.93E+04	7.36E-04
82	4.09E+04-4.63E+04	4.74E+00	4.35E+04	8.71E-04
83	3.43E+04-4.09E+04	6.06E+00	3.74E+04	9.24E-04

Table F8.2.1 (continued)

Group	Limits	Flux	Average energy	Flux per unit energy
84	3.18E+04-3.43E+04	2.14E+00	3.30E+04	8.63E-04
85	2.85E+04-3.18E+04	1.81E+00	3.01E+04	5.44E-04
86	2.70E+04-2.85E+04	7.37E+00	2.77E+04	4.91E-03
87	2.61E+04-2.70E+04	1.36E+00	2.65E+04	1.44E-03
88	2.48E+04-2.61E+04	2.34E+00	2.54E+04	1.84E-03
89	2.36E+04-2.48E+04	1.68E+00	2.42E+04	1.39E-03
90	2.19E+04-2.36E+04	2.36E+00	2.27E+04	1.38E-03
91	1.93E+04-2.19E+04	3.96E+00	2.05E+04	1.54E-03
92	1.50E+04-1.93E+04	6.82E+00	1.70E+04	1.60E-03
93	1.17E+04-1.50E+04	5.66E+00	1.33E+04	1.70E-03
94	9.12E+03-1.17E+04	4.86E+00	1.03E+04	1.88E-03
95	7.10E+03-9.12E+03	3.27E+00	8.05E+03	1.62E-03
96	5.53E+03-7.10E+03	3.08E+00	6.27E+03	1.96E-03
97	4.31E+03-5.53E+03	2.38E+00	4.88E+03	1.95E-03
98	3.71E+03-4.31E+03	9.11E-01	4.00E+03	1.52E-03
99	3.35E+03-3.71E+03	3.85E-01	3.53E+03	1.09E-03
100	3.04E+03-3.35E+03	1.93E-01	3.19E+03	6.05E-04
101	2.75E+03-3.04E+03	8.84E-02	2.89E+03	3.06E-04
102	2.61E+03-2.75E+03	5.17E-02	2.68E+03	3.86E-04
103	2.03E+03-2.61E+03	9.60E-01	2.31E+03	1.66E-03
104	1.58E+03-2.03E+03	1.97E+00	1.80E+03	4.38E-03
105	1.23E+03-1.58E+03	2.04E+00	1.40E+03	5.82E-03
106	9.61E+02-1.23E+03	1.53E+00	1.09E+03	5.60E-03
107	7.49E+02-9.61E+02	1.17E+00	8.48E+02	5.50E-03
108	4.54E+02-7.49E+02	1.44E+00	5.83E+02	4.89E-03
109	2.14E+02-4.54E+02	7.72E-01	3.12E+02	3.22E-03
110	1.01E+02-2.14E+02	1.97E-01	1.47E+02	1.74E-03
111	4.79E+01-1.01E+02	2.89E-02	6.96E+01	5.41E-04
112	2.26E+01-4.79E+01	2.91E-03	3.29E+01	1.15E-04
113	1.07E+01-2.26E+01	2.45E-04	1.55E+01	2.05E-05
114	5.04E+00-1.07E+01	2.03E-05	7.34E+00	3.60E-06
115	2.38E+00-5.04E+00	2.14E-06	3.47E+00	8.04E-07
116	1.13E+00-2.38E+00	7.86E-07	1.64E+00	6.25E-07
117	4.14E-01-1.13E+00	6.02E-08	6.83E-01	8.46E-08
118	1.00E-01-4.14E-01	8.22E-09	2.03E-01	2.62E-08
119	1.00E-05-1.00E-01	1.98E-09	1.00E-03	1.98E-08

On the other hand, the P_ℓ matrices are Legendre coefficients for a fit to the group-to-group term, normalized such that $f_0(i \rightarrow j) = 1.0$, and consistent with the probabilities in the P_0 data. Therefore, if one wanted a value for the cross section through a particular scattering angle whose cosine is μ for the group i to group j transfer for a mixture with order NL matrices:

$$\Sigma(i \rightarrow j,\mu) = \Sigma(i,MT=2002 \text{ or } 2502)P_0(i \rightarrow j)\left[\frac{1}{2} + \sum_{\ell=1}^{NL} \frac{2\ell+1}{2} f_\ell(i \rightarrow j)P_\ell(\mu)\right],$$

where $P_\ell(\mu)$ is the Legendre polynomial and the f_ℓ are the terms in the matrices.

The probabilities and angles given in the group/angle matrices discussed in Sect. F8.1.4 are selected by techniques based on generalized Gaussian quadratures described in Sect. F9.D.2. The probabilities are independent of the group-to-group values mentioned previously and will sum to one over all angles for any transfer. The exception to this rule is when a particular transfer is isotropic in its LAB values, in which case the probability value for the initial angle record will be -1.0, to signal this special situation.

F8.3 PROGRAMMING DETAILS

This section is used to describe the various input/output devices that may be required by ICE and also to describe each of the subroutines in the program.

F8.3.1 INPUT/OUTPUT DEVICE SPECIFICATIONS

The following devices are typically needed in running ICE:

Logical Number	
3	AMPX working library output unit.
4	AMPX working library input unit.
7	Punched card output unit.
8	Direct-access scratch device.*
9	Direct-access scratch device.*
14	Monte Carlo processed cross-section library output unit.
20	ANISN output unit.
21	ANISN group-independent output unit.

F8.3.2 SUMMARY OF FUNCTIONS BY SUBPROGRAM

On the following pages are described the subprograms written specifically for ICE. All are written in FORTRAN. Descriptions of library subprograms shared by more than one SCALE module are given in Sect. M2 of this document. These routines are identified by an asterisk in the list labeled SUBROUTINES CALLED.

F8.3.2.1 BAR

BAR performs initialization functions, reads the title and the first data block, opens the input/output units to be used in the problem, and then calls ALOCAT to dynamically allocate memory to ICE which is the control routine for the rest of the program flow.

---

*Direct-access space is automatically provided on Units 8 and 9 when ICE is used as a module of SCALE or AMPX.

ARGUMENTS:

None

SUBROUTINES CALLED:

MESAGE*, DATIM*, FIDAS*, Q0READ*, DA*, RITE*, REED*, ALOCAT*, CLOSDA*

COMMON BLOCKS:

EXECUT, GIN, BLKLNC, VODKA, SCOTCH, DRTACS

F8.3.2.2 BITTRS

FUNCTION:

BITTRS is called to print an error message and to terminate processing. The message identifies in what part of ICE an error was found, and what corrective action is needed for some errors.

CALLING SEQUENCE:

CALL BITTRS(KEY)

ARGUMENTS:

KEY is the variable identifying which error occurred.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

VODKA

F8.3.2.3 CHERRY

FUNCTION:

CHERRY finds the roots of a polynomial by an interval-halving technique.

CALLING SEQUENCE:

CALL CHERRY(L,NF)

ARGUMENTS:

L is the number of roots to be found.
NF is an error flag returned to the calling program.

0 is no error.
1 is an error occurred in trying to find the roots.

SUBROUTINES CALLED:

CREAM

COMMON BLOCKS:

VODKA, COGNAC, BOURBN

F8.3.2.4 COKE

FUNCTION:

COKE uses the magic word arrays to calculate the pointer into a transfer array for a given transfer.

CALLING SEQUENCE:

CALL COKE(MWA,IG,IGF,J,IND)

ARGUMENTS:

MWA is the magic word array.
IG is the sink group for the transfer.
IGF is the source group for the transfer.
J is the mixture number of the transfer array.
IND is the pointer into the array returned by COKE.
IND is returned as -1 if the requested transfer does not exist.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

GIN, VODKA

F8.3.2.5 CREAM

FUNCTION:

CREAM evaluates the orthogonal polynomials used to calculate the discrete angles and probabilities for the Monte Carlo library.

CALLING SEQUENCE:

POLY CREAM(ND,X)

ARGUMENTS:

ND is the order of the polynomial to be evaluated.
X is the value of the independent variable at which the polynomial is to be evaluated.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

TEQILA

F8.3.2.6 DTFPUN

FUNCTION:

DTFPUN is used to punch the ANISN-formatted mixed cross sections in a FIDO fixed-format scheme which can be read by a FIDO input routine.

CALLING SEQUENCE:

CALL DTFPUN(E,N,R,ISUM,NCARD)

ARGUMENTS:

E	is the array of variables to be punched on the next card.
N	is the array of repeat factors corresponding to each value of E.
R	is an array of characters for each entry, E. A blank means no repeats, an R means N repeats.
ISUM	is the number of entries in E (<7).
NCARD	is the sequence number to be punched in columns 73-80.

SUBROUTINES CALLED:

FLTFX*

COMMON BLOCKS:

None

F8.3.2.7 GJ

FUNCTION:

GJ is used to read the 1-D cross-section arrays from the direct-access scratch unit.

CALLING SEQUENCE:

CALL GJ(SIG,SIG,NRD,NIDS,MSTRT,NNGA,LGTH,NID)

ARGUMENTS:

SIG	is the array into which the cross sections will be read.
GJ	picks up the second occurrence of SIG as an integer array to insert the identifiers of the 1-D cross sections.
NRD	is the array containing the direct-access pointers for each cross-section block.
NIDS	is the number of 1-D arrays.
MSTRT	is the offset in the NRD array to the pointers for the cross sections.
NNGA	is the number of energy groups.
LGTH	is the first dimension of SIG (NNGA+1).
NID	is the array containing the cross-section identifiers.

SUBROUTINES CALLED:

REED*

COMMON BLOCKS:

DRTACS

F8.3.2.8 GUAVAJ

FUNCTION:

GUAVAJ is used to convert the mixed P_n scattering arrays into probabilities and angles for use by Monte Carlo codes.

CALLING SEQUENCE:

CALL GUAVAJ(SIG,NCOEF,MWB,NRD,NRA,MWD,NMTG,NRE,NSPACE)

ARGUMENTS:

SIG	is a two-dimensional (2-D) array used for reading in and normalizing the P_n coefficients and for storing the angles and probabilities until they are written out on disk.
NCOEF	is the array containing the number of coefficients to be saved for each mixture.
MWB	is the array containing the pointers for the primary-to-primary and the secondary-to-secondary transfers by mixture.
NRD	is the array containing the direct-access pointers for the P_n coefficient arrays.
NRA	is the array where the direct-access pointers to the angles and probabilities are stored.
MWD	is the array containing the pointers for the primary-to-secondary transfers if the cross sections are not fully coupled.
NMTG	is the total number of energy groups.
NRE	is a temporary array used to hold direct-access pointers to the angles and probabilities while they are being created.
NSPACE	is the amount of space available for constructing angles and probabilities.

SUBROUTINES CALLED:

SOURMX, REED*, RITE*, RD*

COMMON BLOCKS:

DRTACS, RUM, VODKA, GIN, WHISKY, BOURBN, TEQILA

F8.3.2.9 ICE

FUNCTION:

ICE controls the major flow of the program. It sets up pointers and calls routines to perform the major functions requested by the input.

CALLING SEQUENCE:

CALL ICE(D,LIM)

ARGUMENTS:

D	is a scratch array used for variably dimensioning the arrays needed by ICE.
LIM	is the number of words of storage available in D.

SUBROUTINES CALLED:

OJ, PJ, TJ, LIME, PEEL, PICK, QUI9, SODA, LEMON, SPILL, TONIC, BITTRS, GUAVAJ, SELTZR, SEVNUP, SHAKER, SPRITE, SWIZLE, TABSCO, FIDAS*, Q0READ*

COMMON BLOCKS:

EXECUT, GIN, VODKA, SCOTCH, RUM

F8.3.2.10 LEMON

FUNCTION:

LEMON loops over the mixtures and calls TWIST to make an ANISN binary cross-section library.

CALLING SEQUENCE:

CALL LEMON(D,ANSN,S1D,MWA,NRC,NID,NGD,NCOEFF,MAD,IMT,KID,KGD)

ARGUMENTS:

D	is a scratch array used to read in the cross sections in a magic word format.
ANSN	is the array in which the ANISN-ordered cross sections are stored before they are written out.
S1D	is the scratch array used to read in the 1-D cross sections.
MWA	is the array containing the pointers into the transfer arrays.
NRC	is the array containing the direct-access pointers to the mixed cross sections.
NID	is the array containing the identifiers of the 1-D neutron cross sections in the mixed library.
NGD	is the array containing the identifiers of the 1-D gamma cross sections in the mixed library.
NCOEF	is the array containing the number of coefficients for each mixture to be output on the ANISN library.
MAD	is the array containing the identifiers for each cross-section set on the ANISN library.
IMT	is the array containing the identifiers of the 1-D cross sections to be output on the ANISN library.
KID	is a temporary array used in putting in the 1-D neutron cross sections into the ANISN library.
KGD	is a temporary array used in putting in the 1-D gamma cross sections into the ANISN library.

SUBROUTINES CALLED:

TWIST

COMMON BLOCKS:

GIN, SCOTCH, VODKA

F8.3.2.11 LIME

FUNCTION:

LIME is called to compute the length of a single group of cross sections on an ANISN group-independent library.

CALLING SEQUENCE:

CALL LIME(LMAX,MIX,LMAXMX,NCOEF)

ARGUMENTS:

LMAX	is the table length of the ANISN cross sections.
MIX	is the number of mixtures to go on the group-independent library.
LMAXMX	is the length of a single group on the group-independent library.
NCOEF	is an array of the number of P_n coefficients for each mixture.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

None

F8.3.2.12 MAIN

FUNCTION:

MAIN is the main program for ICE when it is run in the "stand-alone" mode. It sets the input mode to read cards and calls BAR.

CALLING SEQUENCE:

None

ARGUMENTS:

None

SUBROUTINES CALLED:

BAR

COMMON BLOCKS:

EXECUT

F8.3.2.13 Q#$007

FUNCTION:

Q#$007 is the main program for ICE when it is run as a module in the SCALE system. It sets the input mode to read a binary interface and call BAR.

CALLING SEQUENCE:

None

ARGUMENTS:

None

SUBROUTINES CALLED:

BAR

COMMON BLOCKS:

EXECUT

F8.3.2.14 OJ

FUNCTION:

OJ calculates the pointer arrays into the transfer arrays for the neutron-to-neutron transfers, neutron-to-gamma transfers, and gamma-to-gamma transfers for the Monte Carlo cross-section library. OJ then reorders the mixed cross-section transfer arrays into forward order and writes them on a scratch unit. It then writes the 1-D cross sections on the scratch unit.

CALLING SEQUENCE:

CALL OJ(SIG,BUF,NRC,NRD,MWA,MWB,MWC,NCOEF,NID,NGD)

ARGUMENTS:

SIG	is a scratch array used to read and write the cross sections.
BUF	is a scratch array used in reordering the cross sections.
NRC	is the array holding the pointers to the mixed cross sections on the random-access scratch unit.

NRD	is the array in which the pointers to the Monte Carlo cross sections on the random-access scratch unit are saved.
MWA	is the magic word pointer array into the input cross-section arrays.
MWB	is the magic word pointer array into the Monte Carlo neutron-to-neutron and gamma-to-gamma cross-section arrays.
MWC	is the magic word pointer array into the Monte Carlo neutron-to-gamma cross-section arrays.
NCOEF	is the arrays giving the number of P_n coefficients for each mixture.
NID	is the array containing the identifiers of the different 1-D neutron cross sections.
NGD	is the array containing the identifiers of the different 1-D gamma cross sections.

SUBROUTINES CALLED:

BITTERS, COKE, REED*, RITE*

COMMON BLOCKS:

GIN, RUM, VODKA, DRTACS

F8.3.2.15 OLIVE

FUNCTION:

OLIVE converts a set of Legendre coefficients to moments of the distribution, calls PEPSI to calculate the parameters of the orthogonal polynomials for that set of moments, and then OLIVE calculates the angles and probabilities for the distribution.

CALLING SEQUENCE:

CALL OLIVE(IG1,JG1,MX,INUSN)

ARGUMENTS:

IG1	is the source group for the transfer.
JG1	is the index to the current transfer.
MX	is the current mixture number.
INUSN	is a count of the number of errors.

SUBROUTINES CALLED:

CHERRY, CREAM, ONION, PEPSI

COMMON BLOCKS:

VODKA, GIN, RUM, COGNAC, TEQILA, BOURBN, WHISKY

F8.3.2.16 ONION

FUNCTION:

ONION calculates and prints diagnostic information for a scattering distribution with invalid moments.

CALLING SEQUENCE:

CALL ONION

ARGUMENTS:

None

SUBROUTINES CALLED:

CREAM, RC

COMMON BLOCKS:

VODKA, WHISKY, TEQILA, COGNAC

F8.3.2.17 PEEL

FUNCTION:

PEEL constructs and writes the group-independent cross-section library (GIP).

CALLING SEQUENCE:

CALL PEEL(ANSN, SIG, S1D, MWA, NRC, NID, NGD, NCOEF, LMAX, NOGP, LMAXMX, IMT, KID, KGD)

ARGUMENTS:

ANSN	is the array in which the cross sections are stored before being written on the group-independent tape.
SIG	is the array into which the mixed cross sections are read.
S1D	is the array into which the 1-D mixed cross sections are read.
MWA	is the magic word pointer array into the mixed cross-section transfer arrays.
NRC	is the pointer array to the mixed cross sections on the random-access scratch unit.
NID	is the array containing the identifiers for the 1-D mixed neutron cross sections.
NGD	is the array containing the identifiers for the 1-D mixed gamma cross sections.
NCOEF	is the array containing the number of P_1 coefficients each mixture has.
LMAX	is the length of one group and mixture of cross sections.
NOGP	is the number of groups of cross sections that can be held in memory at one time.

LMAXMX	is the length of the group-independent cross-section string.
IMT	is the array containing the identifiers of the 1-D cross sections to be output on the group-independent library.
KID	is an array containing the correspondence between the input and output 1-D neutron cross sections.
KGD	is an array containing the correspondence between the input and output 1-D gamma cross sections.

SUBROUTINES CALLED:

FFPUN*, PUNSH, REED*

COMMON BLOCKS:

GIN, VODKA, DRTACS

F8.3.2.18 PEPPER

FUNCTION:

PEPPER is used to adjoint the neutron-to-gamma cross sections if needed before they are written on the Monte Carlo library.

CALLING SEQUENCE:

CALL PEPPER(S,T,MWE,MWC,MG)

ARGUMENTS:

S	is the array containing the neutron-to-gamma cross sections.
T	is a buffer array used in inverting the cross sections.
MWE	is the array containing the pointers to the cross sections in S upon entry to PEPPER.
MWC	is the array containing the pointers to the inverted S when exiting PEPPER.
MG	is the number of groups in MWE.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

VODKA, RUM

F8.9.2.19 PEPSI

FUNCTION:

PEPSI uses the moments of a scattering distribution to calculate the parameters of the orthogonal polynomials having the distribution as the weighting function.

CALLING SEQUENCE:

CALL PEPSI

ARGUMENTS:

None

SUBROUTINES CALLED:

None

COMMON BLOCKS:

VODKA, WHISKY, TEQILA, COGNAC

F8.3.2.20 PICK

FUNCTION:

PICK is used to truncate the transfer arrays when requested by the input.

CALLING SEQUENCE:

CALL PICK(SIG,SIGN,MWA,MWB,NRC,NR,NCOEF)

ARGUMENTS:

SIG	is the buffer array used to read the cross sections into.
SIGN	is the buffer array used to hold the truncated cross sections.
MWA	contains the pointers to the untruncated arrays.
MWB	contains the pointers to the truncated arrays.
NRC	contains the block pointers to the data on the input random-access unit.
NR	contains the block pointers to the data on the output random-access unit.
NCOEF	contains the number of P_n coefficients for each mixture.

SUBROUTINES CALLED:

COKE, REED*, RITE*

COMMON BLOCKS:

GIN, VODKA, DRTACS

F8.3.2.21 PJ

FUNCTION:

PJ is used to invert the cross sections for an adjoint Monte Carlo library. It then calculates the 1-D cross sections representing the sum of the transfers to untruncated groups and to truncated groups.

CALLING SEQUENCE:

CALL PJ(SIG, BUF, NRD, MWA, MWB, MWC, NCOEF, NID, NGD, MWD, MWE, MWF, NMTG, MG)

ARGUMENTS:

SIG	is the array used to hold the cross sections.
BUF	is a scratch array.
NRD	is the array of random-access pointers to the cross sections.
MWA	is the array containing pointers into the neutron-to-neutron and the gamma-to-gamma transfer arrays.
MWB	contains the pointers into the inverted arrays.
MWC	contains the pointers into the neutron-to-gamma arrays.
NCOEF	contains the number of P_n coefficients for each mixture.
NID	contains the identifiers of the neutron 1-D cross sections.
MWD	contains the pointers into the inverted neutron-to-gamma arrays.
NGD	contains the identifiers of the gamma 1-D cross sections.
MWE	contains the initial pointers into the neutron to gamma arrays.
MWF	is set to MWB upon exit from PJ.
NMTG	is the total number of groups.
MG	is the number of neutron groups.

SUBROUTINES CALLED:

SALT, PEPPER, SUGAR, REED*, RITE*

COMMON BLOCKS:

GIN, RUM, VODKA, DRTACS

F8.3.2.22 PUNSH

FUNCTION:

PUNSH sets up each card to be punched by DTFPUN in fixed-FIDO format.

CALLING SEQUENCE:

CALL PUNSH(X, N)

ARGUMENTS:

X is the array of data to be punched.
N is the number of elements of X to be punched.

SUBROUTINES CALLED:

DTFPUN

COMMON BLOCKS:

None

F8.3.2.23 QUI9

FUNCTION:

QUI9 writes the mixed AMPX working library.

CALLING SEQUENCE:

CALL QUI9(SIG, ISIG, SID, ISID, SIGO, MWA, NCOEF, NRC, NID, NGD, LGH, MID)

ARGUMENTS:

SIG	is a scratch array used for reading and writing.
ISIG	is the same array as SIG, but defined as an integer array.
SID	is an array used to hold the ID record for a nuclide.
ISID	is the same array as SID, but defined as an integer array.
SIGO	is a scratch array used to read the transfer arrays into before the magic words are added.
MWA	is the pointer array for the mixed transfer arrays.
NCOEF	holds the number of P_n coefficients for each mixture.
NRC	contains the random-access pointers for the mixed cross sections.
NID	contains the identifiers for the 1-D neutron cross sections.
NGD	contains the identifiers for the 1-D gamma cross sections.
LGH	is an array used to hold the length of each P_1 array.
MID	is an array containing the identifiers for each nuclide.

SUBROUTINES CALLED:

REED*, RITE*, MGCWRD*, PRTLD*, MWLIST*, RECTRY*

COMMON BLOCKS:

SCOTCH, DRTACS, VODKA, GIN

F8.3.2.24 RC

FUNCTION:

RC is used to convert a set of moments to Legendre coefficients.

CALLING SEQUENCE:

CALL RC(NMO)

ARGUMENTS:

NMO is the number of coefficients to be generated.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

WHISKY

F8.3.2.25 SALT

FUNCTION:

SALT adjoints a 1-D array for the Monte Carlo tape.

CALLING SEQUENCE:

CALL SALT(ARRAY,N)

ARGUMENTS:

ARRAY	is the array to be adjointed.
N	is the number of elements in ARRAY.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

None

F8.3.2.26 SELTZR

FUNCTION:

SELTZR reads the input working library, mixes the cross sections, and writes the mixed cross sections onto a random-access scratch unit for later conversion to the various output libraries.

CALLING SEQUENCE:

CALL SELTZR (SIG, NRC, BUF, IBUF, MWA, RHO, NR, KM, KE, NID, NGD, NCOEF, FNUF, FLUX)

ARGUMENTS:

SIG	is the array the cross sections are mixed in and written out of.
NRC	is the array holding the random-access pointers.
BUF	is a scratch array used to read the input cross sections in to.
IBUF	is the same array as BUF, but typed as an integer array.
MWA	is the array holding the pointers into the transfer arrays.
RHO	is the array of nuclide densities.
NR	is not used.
KM	is the array of mixture numbers.
KE	is the array of nuclide identifiers.
NID	is the array of neutron 1-D cross-section identifiers.
NGD	is the array of gamma 1-D cross-section identifiers.
NCOEF	contains the number of P_n coefficients for each mixture.
FNUF	is a temporary array holding the integral of $\upsilon\Sigma_f\phi$ for each mixture.
FLUX	is the array containing the flux to be used in mixing the fission spectrum.

SUBROUTINES CALLED:

REED*, RITE*, IO*, CLEAR*, MGCWRD*

COMMON BLOCKS:

GIN, VODKA, DRTACS

F8.3.2.27 SEVNUP

FUNCTION:

SEVNUP constructs default values for the 8$, 9$, 10$, and 11$ arrays.

CALLING SEQUENCE:

CALL SEVNUP(MID, MAD, IMT, NCOEF, MUD)

ARGUMENTS:

MID	is the 8$ array.
MAD	is the 9$ array.
IMT	is the 10$ array.
NCOEF	is the 5$ array.
MUD	is the 11$ array.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

GIN, VODKA

F8.3.2.28 SHAKER

FUNCTION:

SHAKER is used to print the Monte Carlo library.

CALLING SEQUENCE:

CALL SHAKER(IOUT, IOT4, BUF, IBUF)

ARGUMENTS:

IOUT	is the logical unit number of the print file.
IOT4	is the logical unit number of the Monte Carlo library.
BUF	is a scratch array used to read the cross sections into for printing.
IBUF	is the same array as BUF, but is typed integer.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

None

F8.3.2.29 SODA

FUNCTION:

SODA is used to read the input library and construct the pointer arrays for the mixture transfer arrays. SODA also determines which 1-D cross sections occur for each mixture and calculates some lengths used to dimension arrays needed later.

CALLING SEQUENCE:

CALL SODA(BUF, IBUF, MWA, KE, KM, IND, NR, NID, NGD, NCOEF)

ARGUMENTS:

BUF	is a scratch work array.
IBUF	is the same array as BUF, but typed integer.
MWA	is the array containing the pointers into the mixed cross-section transfer arrays.
KE	is the array containing the nuclide identifiers.
KM	is the array containing the mixture numbers corresponding to the nuclides in KE.
IND	is a temporary array used to flag that a nuclide has already been processed.
NR	is not used.
NID	is the array containing the identifiers of the 1-D mixed neutron cross sections.
NGD	is the array containing the identifiers of the 1-D mixed gamma cross sections.
NCOEF	is the array containing the number of P_n coefficients for each mixture.

SUBROUTINES CALLED:

BITTRS, IO*, MGCWRD*

COMMON BLOCKS:

GIN, VODKA

F8.3.2.30 SOURMX

FUNCTION:

SOURMX loops over the entries in the mixed transfer arrays constructing the Legendre coefficients for each transfer, and then calls OLIVE to generate the corresponding angles and probabilities.

CALLING SEQUENCE:

CALL SOURMX(SIG, NWRD, NSCT, NPL, NUSED, N1)

ARGUMENTS:

SIG	is a temporary working array containing supergrouped transfer arrays.
NWRD	is the number of different transfers in SIG.
NSCT	is the number of angles to be generated.
NPL	is the number of Legendre coefficients to be generated.
NUSED	is not used.
N1	is not used.

SUBROUTINES CALLED:

OLIVE

COMMON BLOCKS:

WHISKY, BOURBN, TEQILA, DRTACS

F8.3.2.31 SPILL

FUNCTION:

SPILL is used to print out the mixing table and other input data.

CALLING SEQUENCE:

CALL SPILL(KM, KE, RHO, NCOEF, FLUX)

ARGUMENTS:

KM	is the 2$ array.
KE	is the 3$ array.
RHO	is the 4* array.
NCOEF	is the 5$ array.
FLUX	is the 6* array.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

RUM, GIN, VODKA

F8.3.2.32 SPRITE

FUNCTION:

SPRITE is used to generate a default weighting spectrum.

CALLING SEQUENCE:

CALL SPRITE(ENER, L, FLUX)

ARGUMENTS:

ENER	is the array of energy boundaries for the group structure.
L	is the number of groups plus 1.
FLUX	is the defaulted weighting spectrum.

SUBROUTINES CALLED:

LESTER*

COMMON BLOCKS:

VODKA, GIN

F8.3.2.33 SUGAR

FUNCTION:

SUGAR is used to adjoint the neutron-to-neutron and the gamma-to-gamma transfer arrays for a Monte Carlo library.

CALLING SEQUENCE:

CALL SUGAR(SIG, BUF, MWB, MWA, IFTG, NNGA, NMTG)

ARGUMENTS:

SIG	is the array containing the cross sections.
BUF	is a temporary working array.
MWB	contains the pointers into SIG upon entry.
MWA	contains the pointers into the adjointed SIG at exit.
IFTG	is the first thermal group.
NNGA	is the number of neutron groups.
NMTG	is the total number of groups.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

None

F8.3.2.34 SWIZLE

FUNCTION:

SWIZLE loads the correct variables from the 7$ array into common.

CALLING SEQUENCE:

CALL SWIZLE(IN)

ARGUMENTS:

IN is the 7$ array.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

RUM, VODKA

F8.3.2.35 TABSCO

FUNCTION:

TABSCO reads the Monte Carlo data from the random-access scratch unit, constructs some pointer arrays, and writes the Monte Carlo library.

CALLING SEQUENCE:

CALL TABSCO(SIG, ISIG, NCOEF, MWB, NRD, NRA, MWD, NMTG, MW, MUD, NID, NGD)

ARGUMENTS:

SIG	is a temporary working array.
ISIG	is the same array as SIG, but is typed integer.

NCOEF	is the number of P_n coefficients for each mixture.
MWB	is the array of pointers into the neutron-to-neutron and the gamma-to-gamma mixed transfer arrays.
NRD	is the array of random-access pointers to the mixed cross sections.
NRA	is the array of random-access pointers to the angles and probabilities.
MWD	is the array of pointers into the neutron-to-gamma mixed transfer arrays.
NMTG	is the total number of groups.
MW	is the pointer array that is written on the Monte Carlo library.
MUD	is the array of identifiers for each mixture written on the Monte Carlo library.
NID	is the array of identifiers for the mixed 1-D neutron cross sections.
NGD	is the array of identifiers for the mixed 1-D gamma cross sections.

SUBROUTINES CALLED:

GJ, REED*

COMMON BLOCKS:

DRTACS, RUM, VODKA, GIN

F8.3.2.36 TJ

FUNCTION:

TJ is used to truncate the cross sections for the Monte Carlo library if requested, and to construct new pointer arrays.

CALLING SEQUENCE:

CALL TJ(SIG, BUF, NRD, MWA, MWB, MWC, NCOEF, NID, NGD, MWD)

ARGUMENTS:

SIG	is the array into which the truncated transfers are summed.
BUF	is a temporary working array used to hold the transfer arrays.
NRD	is the array of random-access pointers to the cross sections.
MWA	is a temporary array used to hold the pointers before truncation.
MWB	is the pointer array after truncation.
MWC	is the pointer array into the neutron-to-gamma transfer array before truncation.
NCOEF	is the array of the number of P_n coefficients for each mixture.
NID	is the array of identifiers for the 1-D mixed neutron cross sections.
NGD	is the array of identifiers for the 1-D mixed gamma cross sections.
MWD	is the pointer array into the truncated neutron-to-gamma transfer array.

SUBROUTINES CALLED:

REED*, RITE*

COMMON BLOCKS:

GIN, RUM, VODKA, DRTACS

F8.3.2.37 TONIC

FUNCTION:

TONIC reads the title record from the AMPX working library, and scans the mixing table to determine both the number of elements and the number of ANISN identifiers needed.

CALLING SEQUENCE:

CALL TONIC(BUF, IBUF, KE, KTEMP, NCOEF)

ARGUMENTS:

BUF	is a temporary working array used to read the title record into.
IBUF	is the same array as BUF, but is typed integer.
KE	is the mixing table array of nuclide identifiers.
KTEMP	is a temporary array used in counting the number of separate nuclides specified in the mixing table.
NCOEF	is the array of the number of P_n coefficients for each mixture.

SUBROUTINES CALLED:

None

COMMON BLOCKS:

VODKA, GIN, DRTACS

F8.3.2.38 TWIST

FUNCTION:

TWIST converts the mixed cross sections to ANISN format and writes the ANISN library.

CALLING SEQUENCE:

CALL TWIST(J, ANSN, SIG, SID, MWA, NRC, NID, NGD, NPL, IMT, KMAD, MAD, KID, KGD)

ARGUMENTS:

J	is the current mixture number.
ANSN	is the array used to hold the ANISN-formatted cross sections.

SIG	is a temporary working array used to hold the mixed cross sections.
SID	is a temporary working array used to hold the mixed 1-D cross sections.
MWA	is the pointer array into the mixed transfer arrays.
NRC	is the array of random-access pointers to the mixed cross sections.
NID	is the array of identifiers of the 1-D mixed neutron cross sections.
NGD	is the array of identifiers of the 1-D mixed gamma cross sections.
NPL	is the number of P_1 coefficients for this mixture.
IMT	is the identifier array for the 1-D cross sections in the ANISN array.
KMAD	is the index of the current ANISN cross-section set.
MAD	is the array of identifiers for the ANISN library.
KID	is the array of index pointers for the 1-D neutron cross sections in the ANISN library.
KGD	is the array of index pointers for the 1-D gamma cross sections in the ANISN library.

SUBROUTINES CALLED:

PUNSH, FFPUN*, REED*, WOT*

COMMON BLOCKS:

GIN, VODKA, DRTACS

F8.4 INPUT INSTRUCTIONS

The input to ICE uses the FIDO schemes described in Sect. M10. In the descriptions, the number of entries expected in an array is given in square brackets.

****

Card A (20A4)

Title card

Data Block 1

-1$ Direct-Access Specifications [4]

1. NB8 Number of blocks for the first direct-access unit; default 200.
2. NL8 Length in units of 4-byte words of a block for first the direct-access unit; default 880.
3. NB9 Number of blocks for the second direct-access unit; default 400.
4. NL9 Length of a block for the second direct-access unit; default 880.

0$ Logical Unit Specifications for Various Cross-Section Libraries [5]

1. INTAPE Input AMPX working library unit; default 4.
2. IOT1 Output AMPX working library unit; default 3.
3. IOT2 Output ANISN library unit;* default 20.
4. IOT3 Output ANISN group-independent library unit;* default 21.
5. IOT4 Output Monte Carlo processed cross-section library unit; default 14.

1$ Problem Size and Major Options [7]

1. MIX Number of cross-section mixtures to be made.
2. NMIX Number of mixing operations (elements times density operations) to be performed.

---

*If punched output is desired, the unit should be set to 7.

3. IFLAG(L) Set greater than zero if AMPX working library output desired. See options in table; default 0.

4. IFLAG(2) Set greater than zero if ANISN format output desired. See options in table; default 0.

5. IFLAG(3) Set greater than zero if group-independent ANISN output desired. See options in table; default 0.

6. IFLAG(4) Set greater than zero if Monte Carlo processed cross-section library output desired. See options in table; default 0.

7. KOPT Option to be used to calculate χ (chi) of the mixture; default 2.

KOPT = 0, χ of element with the largest sum of $\upsilon(I)\ \Sigma_f(I)\phi(I)$ over all groups is used.

KOPT = 1, χ calculated based on an input flux distribution.

KOPT = 2, χ calculated based on a default thermal reactor flux distribution.

KOPT = 3, χ calculated based on a default fast reactor flux distribution.

KOPT = 4, χ calculated based on the fluxes provided in the input tape for each element in the working library.

T - Terminate Block 1

Table IFLAG Options

Print Options

0	No cross-section printing.
1	Print 1-D cross sections (available only in AMPX working library format).
2	Print 1-D cross sections and P cross sections (not available in ANISN group-independent format).
3	Complete cross-section printing.

Output Options

00	No tape or punch output.
10	Binary tape output.

20	Free-form FIDO punch output (available only in ANISN and group-independent ANISN formats).
30	Fixed-form FIDO punch output (available only in ANISN and group-independent ANISN formats).

IFLAG should be set to the sum of the print option and output option desired.

Data Block 2

2$ [NMIX]

1. (KM(I),I=1,NMIX)	Mixture numbers in the mixture specification table - values range from 1 to MIX.

3$ [NMIX]

1. (KE(I),I=1,NMIX)	Element identifiers for the mixture specification table.

4* [NMIX]

1. (RHO(I),I=1,NMIX)	Atom densities for the mixture specification table.

5$ [MIX]

1. (NCOEF(I),I=1,MIX)	Number of Legendre coefficients, including P_o, to be mixed for each mixture.

6* [NG+4]

1. (FLUX(I),I=1,NG)	Flux to be used in calculation of χ if KOPT = 1; default (FLUX(I) = 1.0, I=1, NG), where NG = number of neutron groups.

NOTE: The four following parameters are required only if KOPT = 2 (i.e., a standard thermal reactor flux is calculated).

2. TEMP	Temperature in Kelvin to be used for Maxwellian distribution; default 300.
3. THETA	Temperature in eV to be used for fission spectrum; default 1.3×10^6.
4. AKT	Number of kT at which 1/E distribution and Maxwellian distribution join; default 5.
5. FCUT	Energy in eV at which fission spectrum and 1/E distribution join; default 67.5×10^3.

7$ [10]

1. IHT — Position of σ_T in ANISN format output; default 3.
2. IHS — Position of within-group scattering in ANISN format output; default IHT plus number of thermal groups.
3. IHM — Table length in ANISN format output; default IHS-1 plus total number of groups.
4. LOPT — Set greater than zero if truncations of cross sections defined by the above parameters are to be applied to the AMPX working library and Monte Carlo processed cross section library also; default 0.
5. NNGA — The number of neutron groups for which Monte Carlo cross sections will be processed; default the number of neutron energy groups on the input library.
6. NGGA — The number of gamma groups for which Monte Carlo cross sections will be processed; default the number of gamma energy groups on the input library.
7. NOPT — Option to be used if energy groups are truncated.

    0 downscatters to missing groups kept.
    1 downscatters to missing groups are summed into last downscatter cross section present.
    2 downscatters to missing groups are dropped; default 0.

8. NSCT — Number of discrete scattering angles calculated; default 0.
9. IADJM — Set greater than zero for an adjoint problem; default 0.
10. NNGTP — Set greater than zero if a completely coupled cross section set is desired; default 0.

T - Terminate Data Block 2

Data Block 3

8$ [MIX] Required only if IFLAG(1) > 0

1. (MID(I),I=1,MIX) — Mixture ID numbers for AMPX working library; default (MID(I)=I,I=1,MIX)

9$ [N] Required only if IFLAG(2) or IFLAG(3) > 0

1. (MAD(I),I=1,N) — ANISN mixture ID numbers. $\sum_{I=1}^{Mix}$ NCOEF(I) ID's are required for each mixture for a total of $\sum_{I=1}^{Mix}$ NCOEF(I)

Default as follows:

P_0 for 1st mixture	ID=100
P_1 for 1st mixture	ID=101
P_2 for 1st mixture	ID=102
.	
.	
.	
P_0 for 2nd mixture	ID=200
P_1 for 2nd mixture	ID=201
.	
.	
.	

10$ [IHT] Required only if IFLAG(2) or IFLAG(3) > 0

1. (IMT(I),I=IHT,1,-1) — ENDF-MT numbers of the ID cross sections to be used in the ANISN cross section tables in **inverted order**; default first five positions:

$1(\sigma_T)$, $1452(\upsilon\sigma_f)$, $27(\sigma_a)$, $18(\sigma_f)$, and $1018(\chi)$.

All other positions: 0

11$ [1+MIX] Required only if IFLAG(4) > 0

1. LID — Monte Carlo processed cross-section library identification number; default 1.

2. (MUD(I),I=1,MIX) — Mixture ID numbers for Monte Carlo processed cross-section library; default (MUD(I)=I, I=1, MIX).

T - Terminate Data Block 3

F8.5 SAMPLE PROBLEM

A simple case has been selected to demonstrate the use of ICE. In this case, it is desired to produce mixture cross sections for UO_2 and H_2O using basic data from the sixteen-group Hansen-Roach SCALE library. Information pertinent to the basic data is given in the following table:

Nuclide	Identifier	Order of Scattering
^{235}U	92235	0
^{238}U	92238	0
O	8016	0
H	1301	1

The atom densities to be used are:

UO_2

$N(^{235}U) = 0.01$ atoms/(barn-cm)
$N(^{238}U) = 0.04$ atoms/(barn-cm)
$N(O) = 0.08$ atoms/(barn-cm)

Water

$N(H) = 0.06$ atoms/(barn-cm)
$N(O) = 0.03$ atoms/(barn-cm)

In the sample case, we have elected to make all four possible kinds of output libraries:

(a) an AMPX working library on logical 61,
(b) an ANISN binary library on logical 62,
(c) an ANISN group-independent library on logical 63, and
(d) a Monte Carlo library on logical 64.

We have selected further to identify UO_2 with a 111 on the AMPX working library, with a 1 on the ANISN library and a 1111 on the Monte Carlo, while using 222, 2, and 2222 for the corresponding identifiers for H_2O. (Note that the P_0 block of ANISN data is identified by a 2 and the P_1 by a 3.)

The KOP T = 2 option for determining a fission spectrum was selected and default values for the parameters used in the option (6* array) were allowed.

For the Monte Carlo library, one angle was selected in the group-angle scattering data. In general, the number of angles should be less than or equal to the order of scattering plus 1 divided by 2.

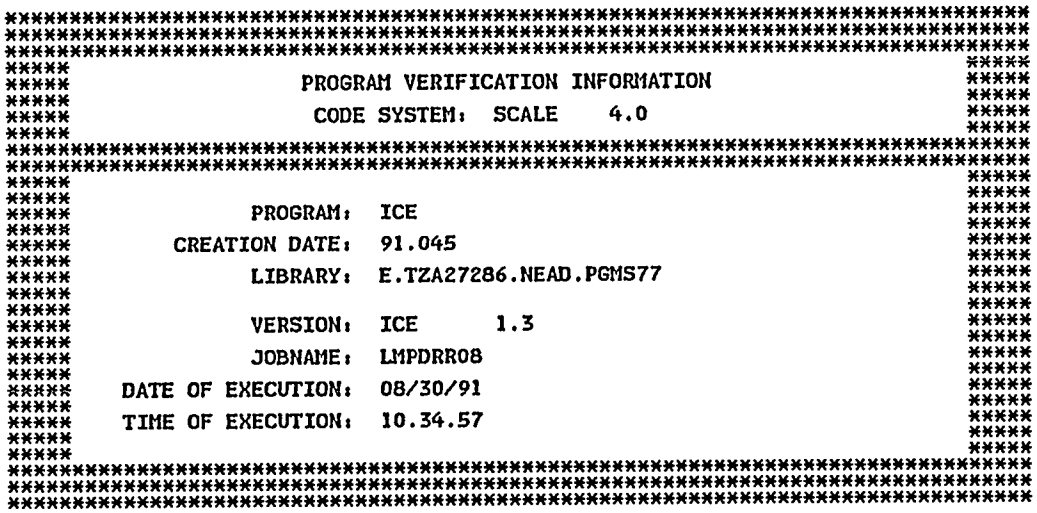
For the ANISN library, the position of the total cross section is 5, while the in-group position is 6, thereby causing any upscatters to be truncated. The table length is 21, which allows a position for all possible downscatters.

NITAWL must be run prior to ICE to produce a working format library for ICE.

A listing of the input data for NITAWL and ICE is as follows:

```
=NITAWL
0$$ 81 E 1$$ A2 4 E 1T
2$$ 1301 8016 92235 92238 2T
END
=ICE
SAMPLE ICE PROBLEM
0$$  4 61 62 63 64
1$$ 2 5 13 13 13 13 2 T
2$$ 3R1 2R2
3$$ 92235 92238 8016 1301 8016
4** 0.01   0.04  0.08 0.06 0.03
5$$ 1 2
7$$ 5 6 21 0 16 0 0 1 0 0
T
8$$ 111 222 9$$ 1 2 3 11$$ 100 1111 2222 T
```

The output produced by ICE is given on the following pages.


PROGRAM VERIFICATION INFORMATION
CODE SYSTEM: SCALE 4.0
PROGRAM: ICE
CREATION DATE: 91.045
LIBRARY: E.TZA27286.NEAD.PGMS77
VERSION: ICE 1.3
JOBNAME: LMPDRR08
DATE OF EXECUTION: 08/30/91
TIME OF EXECUTION: 10.34.57

```
SAMPLE ICE PROBLEM                                                              08/30/91     10.34.57
    0$ ARRAY       5 ENTRIES READ
    1$ ARRAY       7 ENTRIES READ
    1T


 0$ ARRAY
INTAPE          4          IOT3           63
IOT1           61          IOT4           64
IOT2           62


 1$ ARRAY
MIX             2          IFLAG(3)       13
NMIX            5          IFLAG(4)       13
IFLAG(1)       13          KOPT            2
IFLAG(2)       13

    2$ ARRAY       5 ENTRIES READ
    3$ ARRAY       5 ENTRIES READ
    4* ARRAY       5 ENTRIES READ
    5$ ARRAY       2 ENTRIES READ
    7$ ARRAY      10 ENTRIES READ
    2T
 3.000E+02   1.300E+06   5.000E+00   6.750E+04   2.530E-02   1.265E-01   9.275E+03   6.006E-08   9.500E-01   1.500E+07
 3.000E+06   1.400E+06   9.000E+05   4.000E+05   1.000E+05   1.700E+04   3.000E+03   5.500E+02   1.000E+02   3.000E+01
 1.000E+01   3.000E+00   1.000E+00   4.000E-01   1.000E-01


 2$,3$,AND 4* ARRAYS
MIXTURE         1      ELEMENT   92235      DENSITY    0.99999979E-02
MIXTURE         1      ELEMENT   92238      DENSITY    0.39999999E-01
MIXTURE         1      ELEMENT    8016      DENSITY    0.79999983E-01
MIXTURE         2      ELEMENT    1301      DENSITY    0.59999999E-01
MIXTURE         2      ELEMENT    8016      DENSITY    0.29999997E-01


 5$ ARRAY
MIXTURE    1     NO. OF COEFICIENTS     1
MIXTURE    2     NO. OF COEFICIENTS     2


 7$ ARRAY
IHT=        5    IHS=        6    IHM=       21    LOPT=       0
NNGA=      16    NGGA=       0    NOPT=       0    NSCT=       1
IADJM=      0    NNGTP=      0
```

```
WORDS NEEDED TO READ INPUT TAPE=     554
 WORDS CORE NEEDED FOR MIXING=     642
 WORDS AVAILABLE FOR MIXING=  100000

   8$ ARRAY      2 ENTRIES READ
   9$ ARRAY      3 ENTRIES READ
  11$ ARRAY      3 ENTRIES READ

   3T
WORDS NEEDED TO TRUNCATE CROSS SECTIONS=     537

 WORDS CORE NEEDED TO MAKE MIXED AMPX WORKING TAPE=     603
```

1-D NEUTRON CROSS SECTIONS FOR MIXTURE 111

XSEC ID / GRP	1	27	1099	2	101	201	18	102
1	3.08900E-01	4.04428E-02	2.22343E-02	2.66454E-01	3.70136E-03	5.47547E-01	3.67415E-02	5.01356E-04
2	5.15400E-01	3.44000E-02	4.35014E-02	2.81000E-01	2.79354E-03	4.89660E-01	3.16064E-02	2.79354E-03
3	4.84900E-01	1.90600E-02	2.29154E-02	4.65840E-01	5.10232E-03	6.58481E-01	1.39577E-02	5.10232E-03
4	5.52400E-01	1.91000E-02	2.58635E-02	5.33300E-01	7.09999E-03	6.89764E-01	1.20000E-02	7.09999E-03
5	7.03800E-01	2.30000E-02	1.32445E-02	6.80800E-01	8.69918E-03	7.99677E-01	1.43008E-02	8.69918E-03
6	8.64800E-01	4.95000E-02	2.07721E-03	8.15300E-01	2.45000E-02	9.54010E-01	2.50000E-02	2.45000E-02
7	9.95000E-01	8.29999E-02	1.51471E-04	9.12000E-01	4.10000E-02	1.11121E+00	4.20000E-02	4.10000E-02
8	1.10220E+00	1.91000E-01	1.12596E-05	9.11200E-01	1.11980E-01	1.41551E+00	7.90203E-02	1.11980E-01
9	1.54320E+00	7.12000E-01	8.85953E-07	8.31200E-01	5.25000E-01	2.77580E+00	1.87000E-01	5.25000E-01
10	3.33120E+00	2.58000E+00	6.22384E-08	7.51200E-01	2.20000E+00	5.36805E+00	3.80000E-01	2.20000E+00
11	3.78120E+00	3.03000E+00	9.88294E-09	7.51200E-01	2.59367E+00	4.60972E+00	4.36326E-01	2.59367E+00
12	5.89120E+00	5.14000E+00	2.16122E-09	7.51200E-01	4.80286E+00	6.09766E+00	5.37143E-01	4.80286E+00
13	1.15720E+00	4.06000E-01	1.37222E-09	7.51200E-01	1.06000E-01	1.16951E+00	3.00000E-01	1.06000E-01
14	1.57320E+00	8.22000E-01	1.14449E-09	7.51200E-01	1.22000E-01	1.61941E+00	7.00000E-01	1.22000E-01
15	3.03120E+00	2.28000E+00	1.73154E-09	7.51200E-01	4.30000E-01	3.17324E+00	1.85000E+00	4.30000E-01
16	6.95889E+00	6.20761E+00	1.73154E-09	7.51280E-01	1.04762E+00	7.20121E+00	5.16000E+00	1.04760E+00

XSEC ID / GRP	452	1018	16	1452
1	2.84610E+00	2.04000E-01	2.00285E-03	1.04570E-01
2	2.54631E+00	3.44000E-01	0.00000E+00	8.04799E-02
3	2.52119E+00	1.68000E-01	0.00000E+00	3.51900E-02
4	2.49000E+00	1.80000E-01	0.00000E+00	2.98800E-02
5	2.46000E+00	8.99999E-02	0.00000E+00	3.51800E-02
6	2.45000E+00	1.40000E-02	0.00000E+00	6.12500E-02
7	2.45000E+00	0.00000E+00	0.00000E+00	1.02900E-01
8	2.45000E+00	0.00000E+00	0.00000E+00	1.93600E-01
9	2.45000E+00	0.00000E+00	0.00000E+00	4.58149E-01
10	2.45000E+00	0.00000E+00	0.00000E+00	9.30999E-01
11	2.45000E+00	0.00000E+00	0.00000E+00	1.06900E+00
12	2.45000E+00	0.00000E+00	0.00000E+00	8.25999E-01
13	2.45000E+00	0.00000E+00	0.00000E+00	7.35000E-01
14	2.45000E+00	0.00000E+00	0.00000E+00	1.71500E+00
15	2.45000E+00	0.00000E+00	0.00000E+00	4.53250E+00
16	2.45000E+00	0.00000E+00	0.00000E+00	1.26420E+01

P- 0 ARRAY FOR MIXTURE 111

	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
1	1001001	1002002	1003003	1004004	1005005	1006006	6007007	7008008
2	1.31440E-01	1.69820E-01	3.25480E-01	4.61320E-01	6.49840E-01	7.92320E-01	8.88700E-01	8.86700E-01
3		4.98200E-02	5.16800E-02	1.09660E-01	6.79799E-02	3.09600E-02	2.29800E-02	2.33000E-02
4			2.21000E-02	4.51000E-02	2.60000E-02	4.00000E-03		
5				3.81000E-02	3.01000E-02	4.69999E-03		
6					2.56000E-02	4.30000E-03		
7						3.40000E-03		

	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
1	8009009	9010010	10011011	11012012	12013013	13014014	14015015	15016016
2	8.07100E-01	7.17900E-01	7.15180E-01	7.17900E-01	7.15180E-01	7.08460E-01	7.22320E-01	7.51280E-01
3	2.45000E-02	2.41000E-02	3.33000E-02	3.60200E-02	3.33000E-02	3.60200E-02	4.27400E-02	2.88800E-02

1-D NEUTRON CROSS SECTIONS FOR MIXTURE 222

XSEC ID GRP.	1	27	1099	2	101	201
1	1.25940E-01	1.20000E-03	1.53930E-02	1.24740E-01	1.20000E-03	1.71768E-01
2	1.63800E-01	0.00000E+00	3.01164E-02	1.63800E-01	0.00000E+00	2.20962E-01
3	2.99340E-01	0.00000E+00	1.58645E-02	2.99340E-01	0.00000E+00	3.55217E-01
4	3.55080E-01	0.00000E+00	1.79055E-02	3.55080E-01	0.00000E+00	4.40966E-01
5	5.06160E-01	0.00000E+00	9.16926E-03	5.06160E-01	0.00000E+00	6.73966E-01
6	7.99800E-01	0.00000E+00	1.43807E-03	7.99830E-01	0.00000E+00	1.06016E+00
7	9.61500E-01	0.00000E+00	1.04864E-04	9.61500E-01	0.00000E+00	1.27808E+00
8	1.00920E+00	6.00000E-05	7.79509E-06	1.00914E+00	6.00000E-05	1.32806E+00
9	1.00920E+00	2.40000E-04	6.13352E-07	1.00896E+00	2.40000E-04	1.33690E+00
10	1.00920E+00	4.80000E-04	4.30882E-08	1.00872E+00	4.80000E-04	1.33981E+00
11	1.00920E+00	8.40000E-04	6.84204E-09	1.00836E+00	8.40000E-04	1.34015E+00
12	1.00920E+00	1.50000E-03	1.49623E-09	1.00770E+00	1.50000E-03	1.34075E+00
13	1.00920E+00	2.70000E-03	9.49998E-10	1.00650E+00	2.70000E-03	1.36527E+00
14	1.18920E+00	4.20000E-03	7.92340E-10	1.18500E+00	4.20000E-03	1.44365E+00
15	1.60920E+00	7.80000E-03	1.19876E-09	1.60140E+00	7.80000E-03	1.83981E+00
16	2.80924E+00	1.74060E-02	1.19876E-09	2.79183E+00	1.74060E-02	3.09879E+00

P- 0 ARRAY FOR MIXTURE 222

	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
	1001001	1002002	1003003	1004004	1005005	1006006	2007007	3008008
1	2.88600E-02	3.52500E-02	8.14199E-02	1.20960E-01	2.51250E-01	3.55110E-01	4.12590E-01	4.23000E-01
2		5.70600E-02	4.95900E-02	1.33080E-01	1.79760E-01	2.13330E-01	3.68250E-01	4.49970E-01
3			1.38600E-02	4.38600E-02	6.35999E-02	4.51200E-02	3.42600E-02	6.26999E-02
4				1.38600E-02	2.63400E-02	1.76400E-02	7.62000E-03	6.00000E-03
5					8.34000E-03	7.26000E-03	2.94000E-03	1.32000E-03
6						2.76000E-03	1.50000E-03	6.60000E-04
7								

	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
	4009009	5010010	6011011	7012012	8013013	9014014	10015015	11016016
1	4.24440E-01	2.98680E-01	2.69280E-01	2.85960E-01	2.53980E-01	3.78060E-01	1.29147E+00	2.79183E+00
2	4.80900E-01	4.11240E-01	4.76820E-01	5.22060E-01	4.85760E-01	4.56960E-01	6.08940E-01	3.09930E-01
3	8.09399E-02	7.31999E-02	1.15200E-01	1.63140E-01	1.45080E-01	1.41840E-01	2.21040E-01	1.98000E-01
4	1.12200E-02	1.25400E-02	2.16000E-02	4.08000E-02	4.68000E-02	4.31400E-02	7.09199E-02	7.45199E-02
5	1.08000E-03	1.80000E-03	3.66000E-03	7.32000E-03	1.15200E-02	1.39200E-02	2.16000E-02	2.32200E-02
6	3.00000E-04	2.40000E-04	7.50000E-04	1.80000E-03	3.12000E-03	5.76000E-03	9.36000E-03	7.20000E-03
7								

P- 1 ARRAY FOR MIXTURE 222

	GRP. 1	GRP. 2	GRP. 3	GRP. 4	GRP. 5	GRP. 6	GRP. 7	GRP. 8
	1001001	1002002	1003003	1004004	1005005	1006006	2007007	4008008
1	7.20000E-04	2.70000E-03	2.52000E-02	5.02200E-02	3.04740E-01	5.14800E-01	6.15060E-01	6.33060E-01
2		1.00440E-01	1.02420E-01	2.42460E-01	3.15720E-01	3.27780E-01	6.06960E-01	7.47000E-01
3			2.28600E-02	7.66799E-02	8.92799E-02	4.19400E-02	2.28600E-02	4.46400E-02
4				1.71000E-02	2.82600E-02	1.18800E-02	2.88000E-03	1.62000E-03
5					6.29999E-03	3.78000E-03	9.00000E-04	1.80000E-04
6						9.00000E-04	3.60000E-04	
7								

	GRP. 9	GRP. 10	GRP. 11	GRP. 12	GRP. 13	GRP. 14	GRP. 15	GRP. 16
	5009009	6010010	7011011	7012012	8013013	9014014	10015015	11016016
1	6.37560E-01	3.92400E-01	3.26520E-01	3.44700E-01	2.86920E-01	7.20000E-01	1.80000E+00	2.16000E+00
2	7.99920E-01	7.19640E-01	8.93520E-01	9.80099E-01	9.13680E-01	8.89560E-01	1.15200E+00	5.60000E-01
3	5.85000E-02	5.58000E-02	1.14660E-01	1.77660E-01	1.55340E-01	1.61280E-01	2.65320E-01	1.08000E-01
4	3.42000E-03	4.13999E-03	9.18000E-03	2.30400E-02	2.84400E-02	2.73600E-02	4.82400E-02	2.88000E-02
5	1.80000E-04	1.80000E-04	7.20000E-04	1.80000E-03	5.60000E-03	5.04000E-03	8.10000E-03	5.04000E-03
6				1.80000E-04	3.60000E-04	1.08000E-03	1.98000E-03	9.00000E-04
7								

```
      THIS XSDRN WORKING TAPE WAS CREATED 08/30/91 AT 10.34.51
      THE TITLE OF THE PARENT CASE IS AS FOLLOWS
      SCALE 4 - 16 NEUTRON GROUP CRITICALITY SAFETY LIBRARY
        HANSEN-ROACH DATA WITH KNIGHT MODIFICATIONS AND SOME ENDF/B 4 DATA
      MIXED CROSS SECTIONS BY ICE-THE PERFECT MIXER
          TAPE ID                    4016000          NUMBER OF NUCLIDES                  2
          NUMBER OF NEUTRON GROUPS        16          NUMBER OF GAMMA GROUPS              0
          FIRST THERMAL GROUP             13          LOGICAL UNIT                       61
                                  TABLE OF CONTENTS
        MIXED CROSS SECTIONS FROM ICE                                          ID       111
        MIXED CROSS SECTIONS FROM ICE                                          ID       222

          TAPE COPY USED      0 I/O'S, AND TOOK     0.17 SECONDS
AN AMPX WORKING TAPE WAS MADE ON UNIT   61
 HAVE A DRINK
```

WORDS CORE NEEDED TO MAKE ANISN TAPE= 709

NO. OF GROUPS= 16 TBLE LENGTH= 21 CONTROL= 0 ID NO.= 1 TITLE=MIXED CROSS SECTIONS BY ICE-THE PERFECT MIXER

PSN	GRPP 1	GRPP 2	GRPP 3	GRPP 4	GRPP 5	GRPP 6	GRPP 7	GRPP 8
1	2.04000E-01	2.44000E-01	1.68000E-01	1.80000E-01	8.99999E-02	1.40000E-02	0.00000E+00	0.00000E+00
2	3.67415E-02	5.16064E-02	1.39577E-02	1.20000E-02	1.43008E-02	2.50000E-02	4.20000E-02	7.90203E-02
3	4.04428E-02	3.44000E-02	1.90600E-02	1.91000E-02	2.30000E-02	4.95000E-02	8.29999E-02	1.91000E-01
4	1.04570E-01	8.04799E-02	3.51900E-02	2.98800E-02	3.51800E-02	6.12500E-02	1.02900E-01	1.93600E-01
5	3.08900E-01	3.15400E-01	4.84900E-01	5.52400E-01	7.03800E-01	8.64800E-01	9.95000E-01	1.10220E+00
6	1.31440E-01	1.69820E-01	3.25480E-01	4.61320E-01	6.49840E-01	7.92320E-01	8.88700E-01	8.86700E-01
7	0.00000E+00	4.98200E-02	2.16800E-02	1.09660E-01	6.79799E-02	3.09600E-02	2.29800E-02	2.33000E-02
8	0.00000E+00	0.00000E+00	2.21000E-02	4.51000E-02	2.60000E-02	4.00000E-03	0.00000E+00	0.00000E+00
9	0.00000E+00	0.00000E+00	0.00000E+00	3.81000E-02	3.01000E-02	4.69999E-03	0.00000E+00	0.00000E+00
10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.56000E-02	4.30000E-03	0.00000E+00	0.00000E+00
11	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.40000E-03	0.00000E+00	0.00000E+00
12	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	PSN 13 THRU PSN 21 SAME AS ABOVE							

PSN	GRPP 9	GRPP 10	GRPP 11	GRPP 12	GRPP 13	GRPP 14	GRPP 15	GRPP 16
1	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	1.87000E-01	3.80000E-01	4.36326E-01	3.37143E-01	3.00000E-01	7.00000E-01	1.85000E+00	5.16000E+00
3	7.12000E-01	2.58000E+00	3.03000E+00	5.14000E+00	4.06000E-01	8.22000E-01	2.28000E+00	6.20761E+00
4	4.58149E-01	9.30999E-01	1.06900E+00	8.25999E-01	7.35000E-01	1.71500E+00	4.53250E+00	1.26420E+01
5	1.54320E+00	3.33120E+00	3.78120E+00	5.89120E+00	1.15720E+00	1.57320E+00	3.03120E+00	6.95889E+00
6	8.07100E-01	7.17900E-01	7.15180E-01	7.17900E-01	7.15180E-01	7.08460E-01	7.22320E-01	7.51280E-01
7	2.45000E-02	2.41000E-02	3.33000E-02	3.60200E-02	3.33000E-02	3.60200E-02	4.27400E-02	2.88800E-02
8	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	PSN 9 THRU PSN 21 SAME AS ABOVE							

NO. OF GROUPS= 16 TBLE LENGTH= 21 CONTROL= 0 ID NO.= 2 TITLE=MIXED CROSS SECTIONS BY ICE-THE PERFECT MIXER

PSN	GRPP 1	GRPP 2	GRPP 3	GRPP 4	GRPP 5	GRPP 6	GRPP 7	GRPP 8
1	0.00000E+00	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	0.00000E+00	0.00000E+00
3	1.20000E-03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.00000E-05
4	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	1.25940E-01	1.63800E-01	2.99340E-01	3.55080E-01	5.06160E-01	7.99800E-01	9.61500E-01	1.00920E+00
6	2.88600E-02	3.52500E-02	8.14199E-02	1.20960E-01	2.51250E-01	3.55110E-01	4.12590E-01	4.23000E-01
7	0.00000E+00	5.70600E-02	4.95900E-02	1.33080E-01	1.79760E-01	2.13330E-01	3.68250E-01	4.49970E-01
8	0.00000E+00	0.00000E+00	1.38600E-02	4.38600E-02	6.55999E-02	4.51200E-02	3.42600E-02	6.26999E-02
9	0.00000E+00	0.00000E+00	0.00000E+00	1.38600E-02	2.63400E-02	1.76400E-02	7.62000E-03	6.00000E-03
10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.34000E-03	7.26000E-03	2.94000E-03	1.32000E-03
11	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.76000E-03	1.50000E-03	6.60000E-04
12	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	PSN 13 THRU PSN 21 SAME AS ABOVE							

PSN	GRPP 9	GRPP 10	GRPP 11	GRPP 12	CRPP 13	GRPP 14	GRPP 15	GRPP 16
1	0.00000E+00	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	0.00000E+00	0.00000E+00
3	2.40000E-04	4.80000E-04	8.40000E-04	1.50000E-03	2.70000E-03	4.20000E-03	7.80000E-03	1.74060E-02
4	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	1.00920E+00	1.00920E+00	1.00920E+00	1.00920E+00	1.00920E+00	1.18920E+00	1.60920E+00	2.80924E+00
6	4.24440E-01	2.98680E-01	2.69280E-01	2.85960E-01	2.53980E-01	3.78060E-01	1.29147E+00	2.79183E+00
7	4.80900E-01	4.11240E-01	4.76820E-01	5.22060E-01	4.85760E-01	4.56960E-01	6.08940E-01	5.09930E-01
8	8.09399E-02	7.31999E-02	1.15200E-01	1.63140E-01	1.45080E-01	1.41840E-01	2.21040E-01	1.98000E-01
9	1.12200E-02	1.25400E-02	2.16000E-02	4.08000E-02	4.68000E-02	4.31400E-02	7.09199E-02	7.45199E-02
10	1.08000E-03	1.80000E-03	3.66000E-03	7.32000E-03	1.15200E-02	1.39200E-02	2.16000E-02	2.32200E-02
11	3.00000E-04	2.40000E-04	7.50000E-04	1.80000E-03	3.12000E-03	5.76000E-03	9.36000E-03	7.20000E-03
12	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	PSN 13 THRU PSN 21 SAME AS ABOVE							

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NO. OF GROUPS=    16 TBLE LENGTH=    21 CONTROL=     0 ID NO.=     3 TITLE=MIXED CROSS SECTIONS BY ICE-THE PERFECT MIXER

PSN     GRPP  1       GRPP  2       GRPP  3       GRPP  4       GRPP  5       GRPP  6       GRPP  7       GRPP  8
    1  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
       PSN      2 THRU PSN      5 SAME AS ABOVE
    6  7.20000E-04   2.70000E-03   2.52000E-02   5.02200E-02   3.04740E-01   5.14800E-01   6.15060E-01   6.33060E-01
    7  0.00000E+00   1.00440E-01   1.02420E-01   2.42460E-01   3.15720E-01   3.27780E-01   6.06960E-01   7.47000E-01
    8  0.00000E+00   0.00000E+00   2.28600E-02   7.66799E-02   8.92799E-02   4.19400E-02   2.28600E-02   4.46400E-02
    9  0.00000E+00   0.00000E+00   0.00000E+00   1.71000E-02   2.82600E-02   1.18800E-02   2.88000E-03   1.62000E-03
   10  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   6.29999E-03   3.78000E-03   9.00000E-04   1.80000E-04
   11  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   9.00000E-04   3.60000E-04   0.00000E+00
   12  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
       PSN     13 THRU PSN     21 SAME AS ABOVE

PSN     GRPP  9       GRPP 10       GRPP 11       GRPP 12       GRPP 13       GRPP 14       GRPP 15       GRPP 16
    1  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
       PSN      2 THRU PSN      5 SAME AS ABOVE
    6  6.37560E-01   3.92400E-01   3.26520E-01   3.44700E-01   2.86920E-01   7.20000E-01   1.80000E+00   2.16000E+00
    7  7.99920E-01   7.19640E-01   8.93520E-01   9.80099E-01   9.13680E-01   8.89560E-01   1.15200E+00   3.60000E-01
    8  5.85000E-02   5.58000E-02   1.14660E-01   1.77660E-01   1.55340E-01   1.61280E-01   2.65320E-01   1.08000E-01
    9  3.42000E-03   4.13999E-03   9.18000E-03   2.30400E-02   2.84400E-02   2.73600E-02   4.82400E-02   2.88000E-02
   10  1.80000E-04   1.80000E-04   7.20000E-04   1.80000E-03   3.60000E-03   5.04000E-03   8.10000E-03   5.04000E-03
   11  0.00000E+00   0.00000E+00   0.00000E+00   1.80000E-04   3.60000E-04   1.08000E-03   1.98000E-03   9.00000E-04
   12  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
       PSN     13 THRU PSN     21 SAME AS ABOVE
NO. OF GROUPS=     0 TBLE LENGTH=     0 CONTROL=     7 ID NO.=     0 TITLE=MIXED CROSS SECTIONS BY ICE-THE PERFECT MIXER
AN ANISN TAPE WAS MADE ON UNIT   62
 HAVE A DRINK
```

ICE WILL CALCULATE 16 GROUPS OF GROUP INDEPENDENT RECORDS AT A TIME, EACH OF LENGTH 63 WORDS

GROUP= 1

0.2040E+00	0.3674E-01	0.4044E-01	0.1046E+00	0.3089E+00	0.1314E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.1200E-02	0.0000E+00	0.1259E+00	0.2886E-01	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.7200E-03	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00							

GROUP= 2

0.3440E+00	0.3161E-01	0.3440E-01	0.8048E-01	0.3154E+00	0.1698E+00	0.4982E-01	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.1638E+00	0.3525E-01	0.5706E-01	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.2700E-02	0.1004E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00							

GROUP= 3

0.1680E+00	0.1396E-01	0.1906E-01	0.3519E-01	0.4849E+00	0.3255E+00	0.3168E-01	0.2210E-01	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.2993E+00	0.8142E-01	0.4959E-01	0.1386E-01	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.2520E-01	0.1024E+00	0.2286E-01
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00							

GROUP= 4

0.1800E+00	0.1200E-01	0.1910E-01	0.2988E-01	0.5524E+00	0.4613E+00	0.1097E+00	0.4510E-01	0.3810E-01	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.3551E+00	0.1210E+00	0.1331E+00	0.4386E-01	0.1386E-01
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.5022E-01	0.2425E+00	0.7668E-01
0.1710E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00							

GROUP= 5

0.9000E-01	0.1430E-01	0.2300E-01	0.3518E-01	0.7038E+00	0.6498E+00	0.6798E-01	0.2600E-01	0.3010E-01	0.2560E-01
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.5062E+00	0.2512E+00	0.1798E+00	0.6360E-01	0.2634E-01
0.8540E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.3047E+00	0.3157E+00	0.8928E-01
0.2826E-01	0.6300E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00							

GROUP= 6

0.1400E-01	0.2500E-01	0.4950E-01	0.6125E-01	0.8648E+00	0.7923E+00	0.3096E-01	0.4000E-02	0.4700E-02	0.4300E-02
0.3400E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0200E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.7998E+00	0.3551E+00	0.2133E+00	0.4512E-01	0.1764E-01
0.7260E-02	0.2760E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.5148E+00	0.3278E+00	0.4194E-01
0.1188E-01	0.3780E-02	0.9000E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00							

```
 GROUP=      12
  0.0000E+00  0.3371E+00  0.5140E+01  0.8260E+00  0.5891E+01  0.7179E+00  0.3602E-01  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.1500E-02  0.0000E+00  0.1009E+01  0.2860E+00  0.5221E+00  0.1631E+00  0.4080E-01
  0.7320E-02  0.1800E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.3447E+00  0.9801E+00  0.1777E+00
  0.2304E-01  0.1800E-02  0.1800E-03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00
 GROUP=      13
  0.0000E+00  0.3000E+00  0.4060E+00  0.7350E+00  0.1157E+01  0.7152E+00  0.3330E-01  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.2700E-02  0.0000E+00  0.1009E+01  0.2540E+00  0.4858E+00  0.1451E+00  0.4680E-01
  0.1152E-01  0.3120E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2869E+00  0.9137E+00  0.1553E+00
  0.2844E-01  0.3600E-02  0.3600E-03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00
 GROUP=      14
  0.0000E+00  0.7000E+00  0.8220E+00  0.1715E+01  0.1573E+01  0.7085E+00  0.3602E-01  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.4200E-02  0.0000E+00  0.1189E+01  0.3781E+00  0.4570E+00  0.1418E+00  0.4314E-01
  0.1392E-01  0.5760E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.7200E+00  0.8896E+00  0.1613E+00
  0.2736E-01  0.5040E-02  0.1080E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00
 GROUP=      15
  0.0000E+00  0.1850E+01  0.2280E+01  0.4532E+01  0.3031E+01  0.7223E+00  0.4274E-01  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.7800E-02  0.0000E+00  0.1609E+01  0.1291E+01  0.6089E+00  0.2210E+00  0.7092E-01
  0.2160E-01  0.9360E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.1800E+01  0.1152E+01  0.2653E+00
  0.4824E-01  0.8100E-02  0.1980E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00
 GROUP=      16
  0.0000E+00  0.5160E+01  0.6208E+01  0.1264E+02  0.6959E+01  0.7513E+00  0.2888E-01  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.1741E-01  0.0000E+00  0.2809E+01  0.2792E+01  0.3099E+00  0.1980E+00  0.7452E-01
  0.2322E-01  0.7200E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2160E+01  0.3600E+00  0.1080E+00
  0.2880E-01  0.5040E-02  0.9000E-03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00
A GROUP INDEPENDENT ANISN TAPE WAS MADE ON UNIT   63 HAVE A DRINK
     608 WORDS WILL BE USED TO MAKE MORSE/KENO TAPE

     720 WORDS WILL BE USED TO MAKE MORSE/KENO TAPE

     791 WORDS WILL BE USED TO MAKE MORSE/KENO TAPE

MSGPS=    1
     852 WORDS WILL BE USED TO MAKE MORSE/KENO TAPE
```

```
ID RECORD
 100
   1
   0

NEUTRON
ENERGIES AND LETHARGIES
 0.1500E+08  0.3000E+07  0.1400E+07  0.9000E+06  0.4000E+06  0.1000E+06  0.1700E+05  0.3000E+04  0.5500E+03  0.1000E+03
 0.3000E+02  0.1000E+02  0.3000E+01  0.1000E+01  0.4000E+00  0.1000E+00  0.1000E-02 -0.4055E+00  0.1204E+01  0.1966E+01
 0.2408E+01  0.3219E+01  0.4605E+01  0.6377E+01  0.8112E+01  0.9808E+01  0.1151E+02  0.1272E+02  0.1382E+02  0.1502E+02
 0.1612E+02  0.1703E+02  0.1842E+02  0.2303E+02

  12  2  16  0  0  13  16  16  16
   0  0   0  0  0   0   0   0   0
```

```
MIXTURE ID NUMBER 1111
ID RECORD
      1111          0          0          0         47          0          1          0          0         13
         0          0          0          0          0          0          0          0          0          0
         0          0          0          0          0          0          0          0          0          0
         0          6
PRIMARY
ID ARRAYS
         1
  0.3089E+00  0.3154E+00  0.4849E+00  0.5524E+00  0.7038E+00  0.8648E+00  0.9950E+00  0.1102E+01  0.1543E+01  0.3331E+01
  0.3781E+01  0.5891E+01  0.1157E+01  0.1573E+01  0.3031E+01  0.6959E+01
        27
  0.4044E-01  0.3440E-01  0.1906E-01  0.1910E-01  0.2300E-01  0.4950E-01  0.8300E-01  0.1910E+00  0.7120E+00  0.2580E+01
  0.3030E+01  0.5140E+01  0.4060E+00  0.8220E+00  0.2280E+01  0.6208E+01
      1099
  0.2223E-01  0.4350E-01  0.2292E-01  0.2586E-01  0.1324E-01  0.2077E-02  0.1515E-03  0.1126E-04  0.8860E-06  0.6224E-07
  0.9883E-08  0.2161E-08  0.1372E-08  0.1144E-08  0.1732E-08  0.1732E-08
         2
  0.2665E+00  0.2810E+00  0.4658E+00  0.5333E+00  0.6808E+00  0.8153E+00  0.9120E+00  0.9112E+00  0.8312E+00  0.7512E+00
  0.7512E+00  0.7512E+00  0.7512E+00  0.7512E+00  0.7512E+00  0.7513E+00
       101
  0.3701E-02  0.2794E-02  0.5102E-02  0.7100E-02  0.8699E-02  0.2450E-01  0.4100E-01  0.1120E+00  0.5250E+00  0.2200E+01
  0.2594E+01  0.4803E+01  0.1060E+00  0.1220E+00  0.4300E+00  0.1048E+01
       201
  0.5475E+00  0.4897E+00  0.6585E+00  0.6898E+00  0.7997E+00  0.9540E+00  0.1111E+01  0.1416E+01  0.2776E+01  0.5368E+01
  0.4610E+01  0.6098E+01  0.1170E+01  0.1619E+01  0.3173E+01  0.7201E+01
        18
  0.3674E-01  0.3161E-01  0.1396E-01  0.1200E-01  0.1430E-01  0.2500E-01  0.4200E-01  0.7902E-01  0.1870E+00  0.3800E+00
  0.4363E+00  0.3371E+00  0.3000E+00  0.7000E+00  0.1850E+01  0.5160E+01
       102
  0.5014E-03  0.2794E-02  0.5102E-02  0.7100E-02  0.8699E-02  0.2450E-01  0.4100E-01  0.1120E+00  0.5250E+00  0.2200E+01
  0.2594E+01  0.4803E+01  0.1060E+00  0.1220E+00  0.4300E+00  0.1048E+01
       452
  0.2846E+01  0.2546E+01  0.2521E+01  0.2490E+01  0.2460E+01  0.2450E+01  0.2450E+01  0.2450E+01  0.2450E+01  0.2450E+01
  0.2450E+01  0.2450E+01  0.2450E+01  0.2450E+01  0.2450E+01  0.2450E+01
      1018
  0.2040E+00  0.3440E+00  0.1680E+00  0.1800E+00  0.9000E-01  0.1400E-01  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
        16
  0.2003E-02  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
      1452
  0.1046E+00  0.8048E-01  0.3519E-01  0.2988E-01  0.3518E-01  0.6125E-01  0.1029E+00  0.1936E+00  0.4581E+00  0.9310E+00
  0.1069E+01  0.8260E+00  0.7350E+00  0.1715E+01  0.4532E+01  0.1264E+02
      2002
  0.2705E+00  0.2810E+00  0.4658E+00  0.5333E+00  0.6808E+00  0.8153E+00  0.9120E+00  0.9112E+00  0.8312E+00  0.7512E+00
  0.7512E+00  0.7512E+00  0.7512E+00  0.7512E+00  0.7512E+00  0.7513E+00
MWA POINTER ARRAY
         1          7         12         16         19         21         23         25         27         29
        31         33         35         37         40         44          6         11         15         18
        20         22         24         26         28         30         32         34         36         39
        43         47          1          2          3          4          5          6          7          8
         9         10         11         12         13         13         13         13
PRIMARY
P- 0 ARRAY
  0.4860E+00  0.1842E+00  0.8171E-01  0.1409E+00  0.9465E-01  0.1257E-01  0.6043E+00  0.1127E+00  0.1605E+00  0.1071E+00
  0.1530E-01  0.6987E+00  0.2354E+00  0.5581E-01  0.1009E-01  0.8650E+00  0.1275E+00  0.7500E-02  0.9545E+00  0.4548E-01
  0.9718E+00  0.2819E-01  0.9745E+00  0.2555E-01  0.9731E+00  0.2689E-01  0.9710E+00  0.2899E-01  0.9557E+00  0.4433E-01
  0.9521E+00  0.4795E-01  0.9557E+00  0.4433E-01  0.9521E+00  0.4795E-01  0.0000E+00  0.9431E+00  0.5690E-01  0.0000E+00
  0.0000E+00  0.9616E+00  0.3845E-01  0.0000E+00  0.0000E+00  0.0000E+00  0.1000E+01
ANGLE NUMBER 1
  0.4860E+00  0.1842E+00  0.8171E-01  0.1409E+00  0.9465E-01  0.1257E-01  0.6043E+00  0.1127E+00  0.1605E+00  0.1071E+00
  0.1530E-01  0.6987E+00  0.2354E+00  0.5581E-01  0.1009E-01  0.8650E+00  0.1275E+00  0.7500E-02  0.9545E+00  0.4548E-01
  0.9718E+00  0.2819E-01  0.9745E+00  0.2555E-01  0.9731E+00  0.2689E-01  0.9710E+00  0.2899E-01  0.9557E+00  0.4433E-01
  0.9521E+00  0.4795E-01  0.9557E+00  0.4433E-01  0.9521E+00  0.4795E-01  0.0000E+00  0.9431E+00  0.5690E-01  0.0000E+00
  0.0000E+00  0.9616E+00  0.3845E-01  0.0000E+00  0.0000E+00  0.0000E+00  0.1000E+01
PROBABILITY NUMBER 1
 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01
 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01
 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01
 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01
 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01 -0.1000E+01
```

MIXTURE ID NUMBER 2222
ID RECORD

2222	0	0	0	87	1	1	0	0	13
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	7								

PRIMARY
ID ARRAYS

1									
0.1259E+00	0.1638E+00	0.2993E+00	0.3551E+00	0.5062E+00	0.7998E+00	0.9615E+00	0.1009E+01	0.1009E+01	0.1009E+01
0.1009E+01	0.1009E+01	0.1009E+01	0.1189E+01	0.1609E+01	0.2809E+01				
27									
0.1200E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.6000E-04	0.2400E-03	0.4800E-03
0.8400E-03	0.1500E-02	0.2700E-02	0.4200E-02	0.7800E-02	0.1741E-01				
1099									
0.1539E-01	0.3012E-01	0.1586E-01	0.1791E-01	0.9169E-02	0.1438E-02	0.1049E-03	0.7795E-05	0.6134E-06	0.4309E-07
0.6842E-08	0.1496E-08	0.9500E-09	0.7923E-09	0.1199E-08	0.1199E-08				
2									
0.1247E+00	0.1638E+00	0.2993E+00	0.3551E+00	0.5062E+00	0.7998E+00	0.9615E+00	0.1009E+01	0.1009E+01	0.1009E+01
0.1008E+01	0.1008E+01	0.1006E+01	0.1185E+01	0.1601E+01	0.2792E+01				
101									
0.1200E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.6000E-04	0.2400E-03	0.4800E-03
0.8400E-03	0.1500E-02	0.2700E-02	0.4200E-02	0.7800E-02	0.1741E-01				
201									
0.1718E+00	0.2210E+00	0.3552E+00	0.4410E+00	0.6740E+00	0.1060E+01	0.1278E+01	0.1328E+01	0.1337E+01	0.1340E+01
0.1340E+01	0.1341E+01	0.1365E+01	0.1444E+01	0.1840E+01	0.3099E+01				
18									
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00				
102									
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00				
452									
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00				
1018									
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00				
16									
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00				
1452									
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00				
2002									
0.1247E+00	0.1638E+00	0.2993E+00	0.3551E+00	0.5062E+00	0.7998E+00	0.9615E+00	0.1009E+01	0.1009E+01	0.1009E+01
0.1008E+01	0.1008E+01	0.1006E+01	0.1185E+01	0.1601E+01	0.2792E+01				

MWA POINTER ARRAY

1	7	13	19	25	31	37	43	49	55
61	67	72	76	80	84	6	12	18	24
30	36	42	48	54	60	66	71	75	79
83	87	1	2	3	4	5	6	7	8
9	10	11	12	13	13	13	13		

```
PRIMARY
P- 0 ARRAY
  0.2314E+00  0.4574E+00  0.1111E+00  0.1111E+00  0.6686E-01  0.2213E-01  0.2152E+00  0.3027E+00  0.2678E+00  0.1608E+00
  0.4432E-01  0.9158E-02  0.2720E+00  0.4446E+00  0.2125E+00  0.5893E-01  0.9822E-02  0.2205E-02  0.3407E+00  0.5063E+00
  0.1271E+00  0.2146E-01  0.3717E-02  0.8449E-03  0.4964E+00  0.4215E+00  0.6769E-01  0.1185E-01  0.2134E-02  0.4742E-03
  0.4440E+00  0.4604E+00  0.7839E-01  0.1403E-01  0.2250E-02  0.9377E-03  0.4291E+00  0.4680E+00  0.8418E-01  0.1304E-01
  0.3807E-02  0.1872E-02  0.4192E+00  0.4765E+00  0.7254E-01  0.2140E-01  0.7254E-02  0.3092E-02  0.4207E+00  0.4076E+00
  0.1142E+00  0.4044E-01  0.1142E-01  0.5709E-02  0.2961E+00  0.4727E+00  0.1617E+00  0.4640E-01  0.1380E-01  0.9279E-02
  0.2670E+00  0.5177E+00  0.1439E+00  0.4278E-01  0.2142E-01  0.7140E-02  0.2838E+00  0.4820E+00  0.1408E+00  0.7038E-01
  0.2304E-01  0.2523E+00  0.4540E+00  0.2196E+00  0.7404E-01  0.0000E+00  0.3190E+00  0.5139E+00  0.1671E+00  0.0000E+00
  0.0000E+00  0.8065E+00  0.1935E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.1000E+01
P- 1 ARRAY
  0.2495E-01  0.1760E+01  0.1649E+01  0.1234E+01  0.7554E+00  0.3261E+00  0.7660E-01  0.2065E+01  0.1748E+01  0.1073E+01
  0.5207E+00  0.2400E+00  0.3095E+00  0.1822E+01  0.1404E+01  0.6735E+00  0.3061E+00  0.0000E+00  0.4152E+00  0.1756E+01
  0.9295E+00  0.3780E+00  0.1364E+00  0.0000E+00  0.1213E+01  0.1536E+01  0.6673E+00  0.2700E+00  0.1667E+00  0.0000E+00
  0.1450E+01  0.1648E+01  0.7120E+00  0.3048E+00  0.1000E+00  0.0000E+00  0.1491E+01  0.1660E+01  0.7228E+00  0.3301E+00
  0.1967E+00  0.1000E+00  0.1497E+01  0.1663E+01  0.7623E+00  0.4250E+00  0.2459E+00  0.1154E+00  0.1502E+01  0.1750E+01
  0.9953E+00  0.5647E+00  0.3125E+00  0.1875E+00  0.1314E+01  0.1874E+01  0.1089E+01  0.6077E+00  0.3621E+00  0.2115E+00
  0.1213E+01  0.1877E+01  0.1071E+01  0.6342E+00  0.3750E+00  0.1250E+00  0.1205E+01  0.1881E+01  0.1137E+01  0.6802E+00
  0.2171E+00  0.1130E+01  0.1947E+01  0.1200E+01  0.3865E+00  0.0000E+00  0.1904E+01  0.1892E+01  0.5455E+00  0.0000E+00
  0.0000E+00  0.1394E+01  0.1162E+01  0.0000E+00  0.0000E+00  0.0000E+00  0.7737E+00
ANGLE NUMBER  1
  0.8316E-02  0.5868E+00  0.5498E+00  0.4113E+00  0.2518E+00  0.1087E+00  0.2553E-01  0.6884E+00  0.5828E+00  0.3576E+00
  0.1736E+00  0.8000E-01  0.1032E+00  0.6073E+00  0.4679E+00  0.2245E+00  0.1020E+00  0.0000E+00  0.1384E+00  0.5854E+00
  0.3098E+00  0.1260E+00  0.4545E-01  0.0000E+00  0.4043E+00  0.5122E+00  0.2224E+00  0.9000E-01  0.5556E-01  0.0000E+00
  0.4832E+00  0.5494E+00  0.2373E+00  0.1016E+00  0.3333E-01  0.0000E+00  0.4969E+00  0.5534E+00  0.2409E+00  0.1100E+00
  0.6557E-01  0.3333E-01  0.4989E+00  0.5545E+00  0.2541E+00  0.1417E+00  0.8197E-01  0.3846E-01  0.5007E+00  0.5833E+00
  0.3318E+00  0.1882E+00  0.1042E+00  0.6250E-01  0.4379E+00  0.6246E+00  0.3630E+00  0.2026E+00  0.1207E+00  0.7051E-01
  0.4042E+00  0.6258E+00  0.3569E+00  0.2114E+00  0.1250E+00  0.4167E-01  0.4018E+00  0.6270E+00  0.3790E+00  0.2267E+00
  0.7235E-01  0.3766E+00  0.6489E+00  0.4001E+00  0.1288E+00  0.0000E+00  0.6348E+00  0.6306E+00  0.1818E+00  0.0000E+00
  0.0000E+00  0.4646E+00  0.3872E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2579E+00
PROBABILITY NUMBER  1
  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01
  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01  0.1000E+01  0.1000E+01
  0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01
  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01

  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01
  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01
  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01
  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01  0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01
 -0.1000E+01  0.1000E+01  0.1000E+01  -0.1000E+01  -0.1000E+01  -0.1000E+01  0.1000E+01
A MORSE/KENO TAPE WAS MADE ON UNIT   64
 HAVE A DRINK
```

F8.6 REFERENCES

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10. SUPPLEMENTARY NOTES

11. ABSTRACT *(200 words or less)*

SCALE–a modular code system for Standardized Computer Analyses Licensing Evaluation–has been developed by Oak Ridge National Laboratory at the request of the U.S. Nuclear Regulatory Commission. The SCALE system utilizes well-established computer codes and methods within standard analysis sequences that (1) allow an input format designed for the occasional user and/or novice, (2) automate the data processing and coupling between modules, and (3) provide accurate and reliable results. System development has been directed at problem-dependent cross-section processing and analysis of criticality safety, shielding, heat transfer, and depletion/decay problems. Since the initial release of SCALE in 1980, the code system has been heavily used for evaluation of nuclear fuel facility and package designs. This revision documents Version 4.2 of the system.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*
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