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RADHEAT-V3,
A CODE SYSTEM FOR GENERATING COUPLED NEUTRON AND GAMMA-RAY GROUP CONSTANTS AND ANALYZING RADIATION TRANSPORT

July 1977

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RADHEAT-V3, A Code System for Generating Coupled Neutron and Gamma-Ray Group Constants and Analyzing Radiation Transport

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The modular code system RADHEAT is for producing coupled multigroup neutron and gamma-ray cross section sets, analyzing the neutron and gamma-ray transport, and calculating the energy deposition and atomic displacements due to these radiations in a nuclear reactor or shield. The basic neutron cross sections and secondary gamma-ray production data are taken from ENDF/B and POPOP4 libraries respectively.

The system (1) generates multigroup neutron cross sections, energy deposition coefficients and atomic displacement factors due to neutron reactions, (2) generates multigroup gamma-ray cross sections and energy transfer coefficients, (3) generates secondary gamma-ray production cross sections, (4) combines these cross sections into the coupled set, (5) outputs and updates the multigroup cross section libraries in convenient formats for other transport codes, (6) analyzes the neutron and gamma-ray transport and calculates the energy deposition and the number density of atomic displacements in a medium, (7) collapses the cross sections to a broad-group structure, by option, using the weighting functions obtained by one-dimensional transport calculation, and (8) plots, by option, multigroup cross sections, and neutron and gamma-ray distributions.

Definitions of the input data required in various options of the code system are also given.

Keywords : Code System, Coupled Group Constant, Neutron, Gamma-ray, Radiation Transport, Energy Deposition, Cross Sections, Shielding Calculation, Atomic Displacement Factor

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*) Fujitu Ltd.

RADHEAT-V3，中性子-ガンマ線結合群定数作成および放射線輸送解析コードシステム

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RADHEAT-V3は，原子炉及び遮蔽体と，放射線の相互作用を解析するための総合コードシステムであり，中性子に関してはENDF/B，2次ガンマ線生成データに関してはPOPOP 4ライブラリーをそれぞれ基礎データとし中性子とガンマ線の結合群定数を作成し，これを用いて放射線輸送発熱計算を行なう。

このシステムの持つ機能の概要は以下の通りである。

1) 中性子の多群群定数，中性子による発熱定数および放射線損傷につながる原子のはじき出しの割合を与える定数の作成。
2) ガンマ線の輸送群定数と発熱定数の作成。
3) 2次ガンマ線生成断面積の作成。
4) これら定数の結合。
5) 他の輸送計算コード用の多群定数の作成と改訂。
6) 1次元輸送解析による中性子およびガンマ線束の計算，および発熱と原子のはじき出しの計算。
7) 1次元計算による重み関数を用い，2次元輸送計算およびモンテカルロ計算用縮約群定数の作成。
8) 群定数，中性子およびガンマ線束の作図。

この報告は，RADHEAT-V3のユーザーマニュアルとしてまとめたものであり，種々のオプションを使用するために必要な入力データとその定義がまとめられている。

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CONTENTS

Table List

Figure List

1. Introduction

RADHEAT-V3 is a modular code system for producing coupled multigroup neutron and gamma-ray cross section sets, and analyzing the neutron and gamma-ray transport and the atomic displacement in nuclear reactors and shields. This document is a "user's manual" for the system. Therefore, it does not contain detailed discriptions of physics employed in the various modules but describe primarily the input instructions required to select each option available in the RADHEAT-V3.

In the field of reactor physics, the effects of the resonance self-shielding in homogenized mixture, the heterogeneity of cells and the space-dependent spectrum shift in reactors are generally taken into account for generating the multigroup cross sections of neutrons. On the other hand, the cross section set produced under the assumption of fundamental spectrum mode such as 1/E-spectrum has been widely used for shield calculations in most countries, especially in Japan. The characteristics of multigroup cross section set influence directly on the calculational accuracy of the analysis for reactor shields. With the increasing emphasis on the accuracy of shield calculations, the concept adopted in reactor physics will have to be introduced to the generation of the multigroup cross sections in the field of shielding. Moreover, the generation of them has to be carried out with use of the evaluated code system and data base for cross sections at every time when required.

As a code system for generating coupled multigroup neutron and gamma-ray cross sections, a modular code system AMPX[1] developed by N.M. Green, et al. of ORNL is better than the present system in a sense of an easy linkage of a computational module to other modules.

However, the region-wise macroscopic cross sections in a homogenized mixture can not be produced by using the AMPX without taking account of the resonance self-shielding effect which is important as shown in Refs. 2), 3).

In the first version of the RADHEAT[4] system, the computer codes SUPERTOG[5], GAMLEG[6], POPOP4[7] and some codes are joined with each others to generate, in the ANISN format, the neutron and gamma-ray coupled multi-group cross sections and the energy deposition coefficients, from ENDF/B-III and POPOP4 libraries.

Therefore, in planning RADHEAT-V3 as an improved version of the RADHEAT, the following items were considered:

1) To use the ENDF/B libraries which are well evaluated and widely used as

basic cross sections for neutrons.

2) To use the neutron induced gamma-ray library which containes many nuclides and reaction types, and is capable of updating these data.
3) To provide processing codes which have evaluated capabilities as computer codes and can commonly be used.
4) To standardize the format of files produced at each step of the system as much as possible, in order to use them also for sensitivity analyses associated with data and methods for shielding calculations.
5) To automate transferences of data between the computational modules and simplify the preparation of input data.
6) To improve functions of TAPE MAKER as a utility code in order to edit and update the data files produced by the system.
7) To allow, without any restriction, the selection of the execution paths in the system for producing the data required by users.

In addition, the capabilities of the system are expanded by improving the computational modules as follows:

8) To generate directly the energy deposition and the atomic displacement coefficients from ENDF/B libraries.
9) To incorporate the resonance self-shielding effect in a homogenized mixture and the effect of spacial spectrum shift into macroscopic cross sections.
10) To obtain the anisotropic scattering cross sections of gamma rays accurately.

The hierarchy of the RADHEAT-V3 developed under the above considerations is shown in Fig. 1.1. The neutron multigroup cross sections based on the infinite dilution approximation are produced in SUPERTOG-JR3 which is a modified version of SUPERTOG-JR[8] on the cross section format of output file as shown in Appendix F. As an option, user can replace the thermal group cross sections with those generated by using the THERMOS[9] module or the Maxwellian distribution values. This replacement is carried out at the stage between the steps 1 and 2 or at the step 2 shown in Fig. 1.1. In addition, the capabilities producing the energy deposition coefficients and the atomic displacement cross sections for neutrons are provided in SUPERTOG-JR3.

The neutron transport and the secondary gamma-ray production induced by neutron reactions depend directly on the effective cross sections of shielding media, containing especially heavy elements. For producing reasonable and accurate effective cross sections of homogenized mixtures

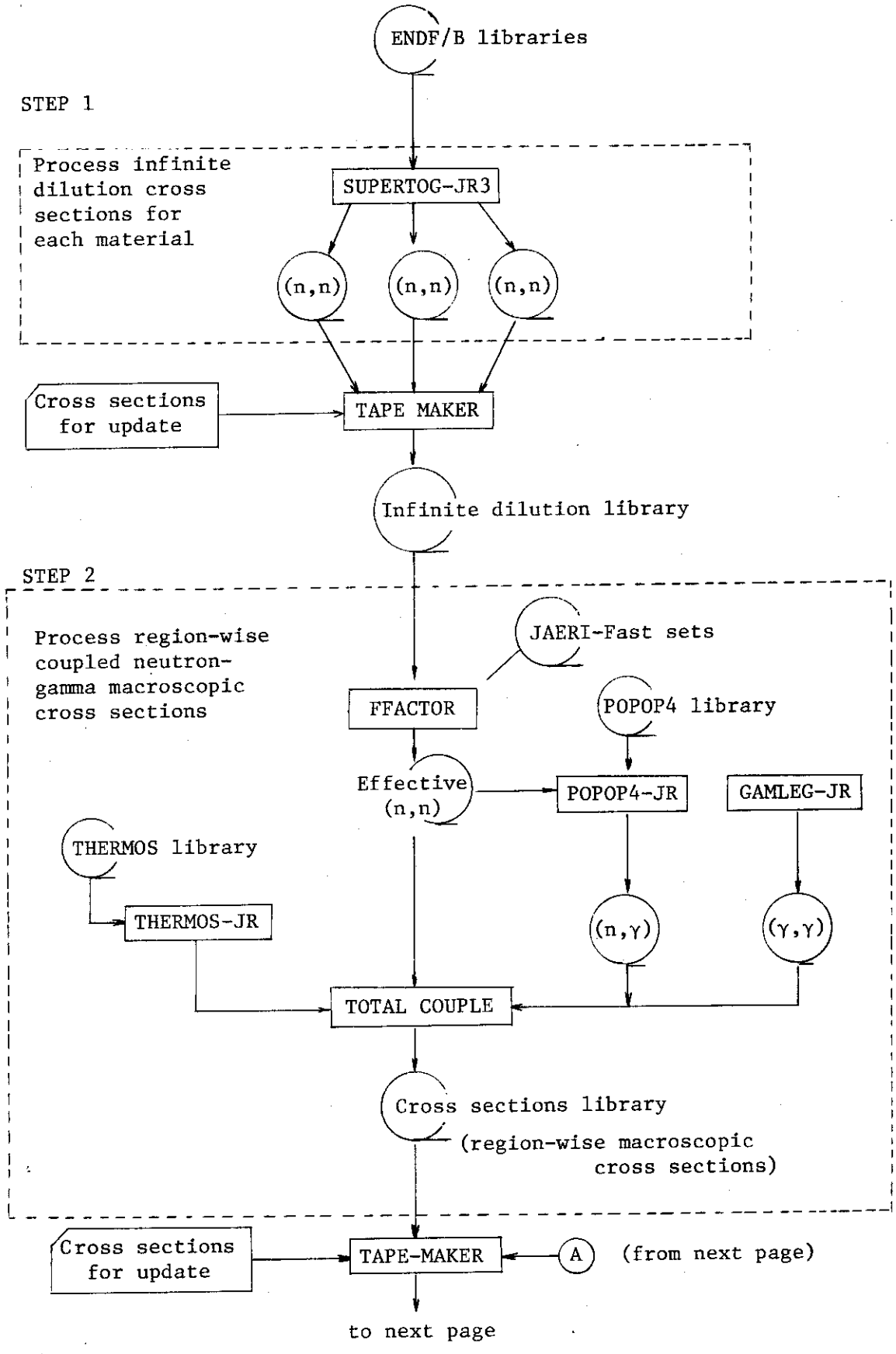

Fig. 1.1 Hierarchy of the code system RADHEAT-V3

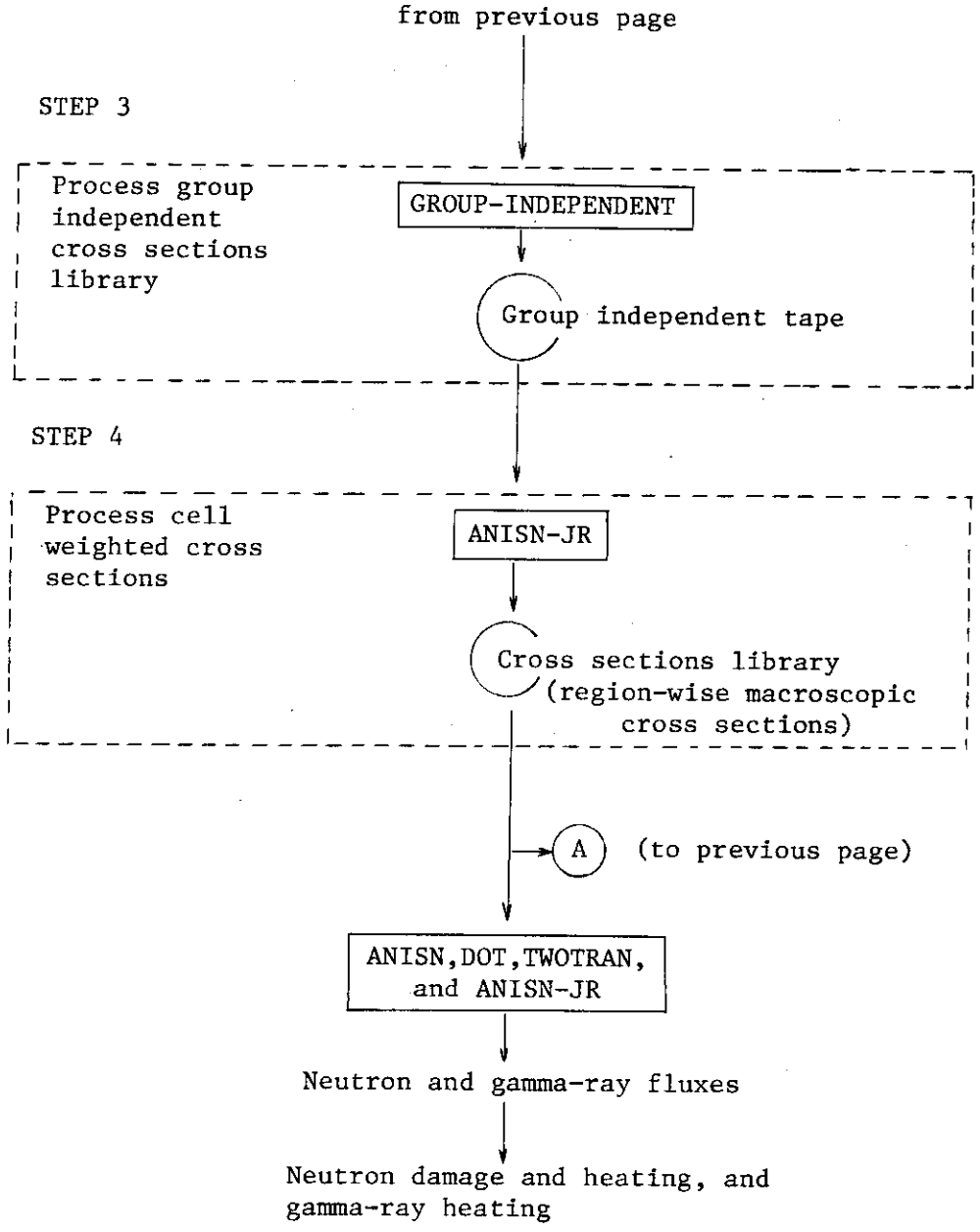

Fig. 1.1 (continued)

in resonance energy regions, we have introduced the self-shielding factors given in the f-table of JAERI-Fast set[10] to the infinite dilution cross sections. The secondary gamma-ray production cross sections are generated from the effective microscopic neutron cross sections for homogenized mixture and the yield data of the POPOP4 library[11].

On the other hand, the effective cross sections for a heterogeneous zone consisting of media of thicknesses of more than several mean free paths should be averaged by using the spectrum in the zone as a weighting function. The ANISN[12] was modified to ANISN-JR[13] so as to produce volume-flux weighted effective cross sections for arbitrary shield zones and regions.

As for photon-absorption cross sections, simple empirical formulas appropriate for machine computations are reported as functions at atomic number Z. Those formulas are introduced to the GAMLEG-JR module[14], so the system can produce the gamma-ray group cross sections by giving only atomic number Z.

The code system includes the following computational modules, descriptions of which are available in the following sections of this document:

(1) CONTROL - Controls all the modules.

(2) SUPERTOG-JR3 - Generates the cross sections for the neutron transport calculation in an infinite dilution approximation, and the energy deposition factor and the atomic displacement factor due to neutron reactions. Also the gamma-ray production cross sections related to POPOP4 are generated.

(3) THERMOS - Generates the cross sections for the thermal neutron group (P_0 components of σ_a, $\nu\sigma_f$, σ_t and $\sigma_{g\to g'}$ and P_1 component of $\sigma_{g\to g'}$).

(4) FFACTOR - Self shielding factors, prepared in the JAERI-Fast set, are multiplied to the cross sections generated in SUPERTOG-JR3.

(5) POPOP4-JR - Generates the secondary gamma-ray yield cross sections. The most reliable data among the POPOP4 library data must be selected.

(6) GAMLEG-JR - Generates the cross sections for the gamma-ray transport calculation.

(7) TOTAL COUPLE - Cross sections for neutrons and gamma-rays are

coupled into the "coupled set". The energy deposition and atomic displacement factors are treated as the activity cross sections in the ANISN format. The coupled sets are kept by a material oriented form as the cross section file.

(8) TAPE MAKER - Collect group cross sections for each element or material produced by the step 1, 2, 3, or ANISN-JR into one file. The updating and copy of libraries and plotting of the data are performed.

(9) GROUP-INDEPENDENT - Selects the necessary materials from the file prepared by TOTAL COUPLE or other files, and transforms them into the group independent form of ANISN-JR.

(10) ANISN-JR*- Analyzes the one-dimensional neutron and gamma-ray transport, and produces the effective cross sections for heterogeneous zones and the collapsed cross sections and detector responses for two-dimensional shield calculations.

The present code system was used for analyzing mockup experiments for the shield modification of the nuclear ship MUTSU,[15),16)] shield benchmark problems given by the NEA[17),18),19)] and benchmark experiments for iron and sodium.[20)] The results have shown an appropriate functioning of the code system.

In the next chapter, we describe the characteristics and input data for MACS (MAcroscopic Cross Section) modules to generate multigroup cross sections for the use in ANISN-JR, input instructions for which are given in Chap. 3. TAPE MAKER is explained in Chap. 4 and four sample problems are shown in Chap. 5 for illustrating the input data.

Note: The form of cross section library generated from RADHEAT-V3 is slightly different from that in the original ANISN on the logical record length to be written on a file as shown in Appendix F.

2. MACS Code Modules

2.1 SUPERTOG-JR3

SUPERTOG-JR3 generates (a) multigroup neutron cross sections for transport calculations, (b) neutron cross sections for secondary gamma-ray productions used in POPOP4-JR module, and (c) heat generation coefficients and atomic displacement cross sections.

These capabilities are the same as in SUPERTOG-JR[8] except for the function (b) to generate independently the cross sections of (n, γ), (n, p), (n, α), (n, n'), (n, 2n), etc. in order to get the cross sections for gamma-ray production due to each reaction. These group cross sections are useful for sensitivity analyses for those reactions. The format of cross section table of SUPERTOG-JR3 is shown in Appendix F.

The details of the capabilities of SUPERTOG-JR are discussed in Ref. 8) and hence we mention them only simply.

The displacement cross sections and heat generation coefficients are generated by the option LINK6 = 1 in SUPERTOG-JR, and are dealt with as the activation cross sections in the code system. Both the coefficients represent the effect of the kinetic energy of neutrons transferring to medium atoms and, therefore, can be generated at the same time in the calculation flow. For the heat generation coefficient, all the kinetic energy transferred to the medium atom is calculated as the energy deposition. On the other hand, for the displacement cross section, only the energy contributing to displace medium atoms in a cascade initiated by a primary knock-on atom is calculated for obtaining the number of displaced atoms. The formulation depends mainly on the Doran's work[21].

In RADHEAT[4], the heat generation coefficient was constructed from the group constant and the group transfer matrices. In the present version, the heat generation coefficient as well as the displacement cross section is generated directly from ENDF/B data.

The general expressions for the displacement cross section F(E) and the heat generation coefficient H(E) at the neutron energy E are written as

$$F(E) = \sigma(E)\int_{E_d}^{T^{max}} \left[\frac{1}{\sigma}\frac{d\sigma(E,\phi)}{d\Omega}\right] \frac{d\Omega}{dT}(E,\phi)\nu(T)dT, \qquad (3.1.1)$$

$$H(E) = \sigma(E)\int_{0}^{T^{max}} \left[\frac{1}{\sigma}\frac{d\sigma(E,\phi)}{d\Omega}\right] \frac{d\Omega}{dT}(E,\phi)T\,dT, \qquad (3.1.2)$$

where $\sigma(E)$ is an appropriate interaction cross section, $d\Omega$ the element of solid angle, ϕ the scattering angle in the center of mass (CM) system, $\nu(T)$ the number of displacement per primary knock-on atom (PKA), T the kinetic energy of PKA in the laboratory system, $T^{max}=\gamma E$ the maximum possible PKA energy corresponding to a head-on collision ($\phi=180°$), and E_d the effective displacement threshold energy.

The integral with respect to μ (cosine of scattering angle) to obtain F(E) is performed with the Gauss-Legendre method. The number of integral points is an input for IMUNO (6$) in the step 1. To calculate the group averaged values $\bar{F}(g)$ and $\bar{H}(g)$, F(E) and H(E) are evaluated at NEPONT points (an input value in 6$ array) for each group. These values are obtained from the following equations:

$$\left.\begin{aligned}\bar{F}(g) &= \int_{E_g}^{E_{g+1}} W(E)F(E)dE \Big/ \int_{E_g}^{E_{g+1}} W(E)dE, \\ \bar{H}(g) &= \int_{E_g}^{E_{g+1}} W(E)H(E)dE \Big/ \int_{E_g}^{E_{g+1}} W(E)dE,\end{aligned}\right\} \qquad (3.1.3)$$

where W(E) is the weighting function.

2.2 THERMOS

THERMOS generates the cross section for thermal neutrons considering the spatial effect of the cell structure, this routine being the same as the original THERMOS[22]. As an option of RADHEAT-V3, the thermal group cross sections (σ_a, σ_f and σ_s for the P_0 and P_1 components) are replaced by those generated in THERMOS from the following form:

$$\bar{\sigma}_R^i = \frac{\int_E \int_V N^i(\vec{\gamma})\sigma_R^i(E)\phi(\vec{\gamma},E)\, d\, dE}{(\int_V N^i(\vec{\gamma}')d\vec{\gamma}' / \int_V d\vec{\gamma}')\int_E \int_V \phi(\vec{\gamma},E)d\vec{\gamma}dE}, \qquad (2.2.1)$$

where

$N^i(\vec{\gamma})$: number density of nucleus i at $\vec{\gamma}$,

$\phi(\vec{\gamma},E)$: neutron flux at $\vec{\gamma}$ and E,

$\sigma_R^i(E)$: microscopic cross section of nucleus i,

R : nuclear reaction type (σ_a, σ_f, σ_{so} for the P_0-component and σ_{s1} for the P_1-component).

In one execution of THERMOS, the cross sections are generated for all

the nuclei i in the cell structure.

2.3 FFACTOR

FFACTOR is a revision of the JFUSER code[23] incorporating the necessary programing changes to produce effective microscopic neutron cross sections in a homogeneous mixture. JFUSER selects required nuclides from the JAERI-Fast 70-group library[10], tabulates the group cross sections of selected nuclides, and produces the collapsed group cross sections from these tables.

The resonance shielding factor is defined by

$$f_R^m(T, \sigma_o) = \frac{\sigma_R^m(\sigma_o)}{\sigma_R^m(\infty)} , \tag{2.3.1}$$

$$\sigma_o = \frac{1}{N^m} \sum_{n \neq m} N^n \sigma_t^n , \tag{2.3.2}$$

where

- m : identification number of nuclide,
- R : identification of reaction type (total, capture, fission or elastic scattering),
- σ_t^m : group averaged total cross section of nuclide m,
- N^m : atomic number density of nuclide m,
- $\sigma_R^m(\infty)$: infinite dilution cross section of nuclide m for reaction type R,
- $\sigma_R^m(\sigma_o)$: effective cross section of nuclide m for reaction type R.

The details of the resonance shielding factor given by Eq.(2.3.1) are discussed in Ref. 10) and hence we mention simply the numerical method. For producing reasonable and accurate resonance cross sections for heavy elements in the JAERI Fast Reactor Group Constant System, the integral kernel of the neutron slowing-down equation in an infinite homogeneous mixture was converted into a recurrence formula. The neutron spectrum was obtained using the recurrence formula for fine narrow groups of equal energy width. From this neutron spectrum and the resonance cross sections, the ABBN type self-shielding factors were obtained.

The resonance shielding factors based on the above definition are

given as the f-table in the JAERI-Fast set for σ_0 = 0, 1, 10, 10^2, 10^3 and 10^4 barns, and for T = 300, 900 and 2100 °K. The required effective microscopic cross sections are calculated by using this f-table. In this calculation, the f-table for the energy group structure of the JAERI-Fast set is converted to that for the requested group structure by interpolating with 1/E spectrum as the weighting function.

The value of σ_0 of a homogeneous medium is obtained from an iterative interpolation method which was used for the ABBN set[24], and the value of σ_t^m for each nuclide in the medium is calculated until the relative deviation of σ_t^m becomes less than one percent by using the MICRO subroutine.

The effective microscopic cross sections obtained from the XRITE subroutine in FFACTOR are read by POPOP4-JR and used for generating the neutron induced gamma-ray production cross sections. The effects of the heterogeneity of a medium on the effective cross sections are not treated by FFACTOR, but can be taken into consideration by ANISN-JR.

2.4 POPOP4-JR

POPOP4-JR is a computational module to generate the neutron induced gamma-ray production cross sections from the POPOP4 library[25] and the effective microscopic neutron cross sections produced by the FFACTOR routine. Its basic calculational algorithm was originally taken from the POPOP4 code[26]. The following modifications were made on POPOP4 to have POPOP4-JR.

1) Changes in management of input/output data files to incorporate into RADHEAT-V3.
2) Automatic read of the neutron cross sections produced by using the FFACTOR code.
3) Restructuring of the input format to incorporate the free-form FIDO input system.

2.5 GAMLEG-JR

The group constants for the photon transport are calculated by using GAMLEG-JR[14] which is a modified version of GAMLEG[6]. In the GAMLEG code, the absorption cross section data for the photoelectric effect, pair production, and coherent scattering are assumed to be given in tabular forms by cards. The GAMLEG-JR generates these cross section data by using the simple empirical formulas[27,28] as a function of atomic number Z. The

module also produces the microscopic gamma-ray heat generation coefficient (KERMA factor).

The KERMA factor is given by

$$h_\gamma(g) = 1.6\times10^{-13}\ (\mu_{en}/\rho)(M/N_0)\bar{E}_g, \quad \text{[barn·watt·sec/atom]} \qquad (2.5.1)$$

where M is the atomic mass number, N_0 is the Avogadro's number, and $\bar{E}_g$ is the mean energy of the g-th group. The (μ_{en}/ρ) is the mass energy-transfer coefficient given by

$$\mu_{en}/\rho = (\frac{C}{\rho})f_C + (\frac{\tau}{\rho})f_\tau + (\frac{\kappa}{\rho})f_\kappa, \qquad (2.5.2)$$

where the first, second, and third terms represent respectively the mass energy-transfer coefficients for Compton scattering, photoelectric absorption and pair production. The code system also calculates the mass energy-transfer coefficient by neglecting the bremsstrahlung effect of recoil electrons.

In the original GAMLEG code, the energy integral of the transfer cross section is performed analytically. The calculation based on this formulation was, however, found not to be adequate for obtaining the cross sections of higher Legendre moments than the 6th order at low energy region below about 0.1 MeV, because of round-off errors due to the machine computation. The present module, GAMLEG-JR, calculates this integral by the numerical integration based on the Simpson's rule for equal spaced $\mu(=1+1/E'-1/E)$.

The calculational method and the results of evaluation for the cross sections are discussed in Ref. 14) in detail.

2.6 TOTAL COUPLE

This module makes a coupled neutron and gamma-ray multigroup cross section table from the neutron cross sections Σ_{nn}, the gamma-ray cross sections $\Sigma_{\gamma\gamma}$, the secondary gamma-ray production cross sections $\Sigma_{n\gamma}$, the neutron and gamma-ray heat generation coefficients H_n and H_γ, and the neutron displacement cross sections D_n produced by using each module mentioned above. The format of the table is shown in Table 2.6.1. Each $P_n(n=1, 2,\ldots,\ell)$ cross section table is in the same form as for the P_0 table. The TAPE MAKER code collects the multigroup cross section table of each element into one library.

Table 2.6.1 Arrangement of group cross section tables for neutrons and gamma rays*

Position	Neutron groups ($1 \leq I \leq ING$)	Gamma-ray groups ($ING+1 \leq J \leq ING+IGG$)
.	$H_n(I)$	$H_\gamma(J)$
.	$D_n(I)$	0.0
.	$\Sigma_a(I)$	$\Sigma_a(J)$
IHT-1	$\nu\Sigma_f(I)$	0.0
IHT	$\Sigma_T(I)$	$\Sigma_T(J)$
IHS	$\Sigma_{nn}(I \to I)$	$\Sigma_{\gamma\gamma}(J \to J)$
IHS+1	$\Sigma_{nn}(I-1 \to I)$	$\Sigma_{\gamma\gamma}(J-1 \to J)$
⋮	⋮	⋮
	$\Sigma_{nn}(1 \to I)$	$\Sigma_{\gamma\gamma}(ING+1 \to J)$
	0.0	$\Sigma_{n\gamma}(ING \to J)$
	⋮	$\Sigma_{n\gamma}(ING-1 \to J)$
	⋮	⋮
	⋮	$\Sigma_{n\gamma}(I \to J)$
	⋮	0.0
. ⋮	⋮	⋮
IHM	⋮	0.0

* ING and IGG are respectively the numbers of neutron groups and gamma-ray groups, and IHM is (IHT+ING+IGG).

2.7 GROUP-INDEPENDENT

This module selects the cross section tables for required materials from the cross section library produced by using the TOTAL COUPLE module, and produces a group independent cross section tape in order to obtain forward or adjoint solutions by ANISN-JR effectively. When this special tape is used, the integer ID2, in the 15$ array of ANISN-JR input, should be set equal to 1. The data area required for ANISN-JR are reduced if this tape is used.

2.8 Input Instruction

The input to MACS code module of RADHEAT-V3 is written in the free-form FIDO format developed by Ward Engle of ORNL, details of which are given in Appendix A. All data with the exception of TITLE cards and THERMOS module are read using the same format. The original FIDO format used in ANISN is also available. To select the free-form, an array is identified with a ** or a $$ depending on whether it is floating or integer array. In the following, the array dimension is given in square blackets, and the condition under which the array is to be specified is given in parentheses. The array without the condition should always be specified.

A. Control Parameters

1$ Main parameter [5]

1. ISTEP selection of the calculational step
   - 1 — STEP1 (SUPERTOG-JR3)
   - 2 — STEP2 (THERMOS, FFACTOR, POPOP4, GAMLEG-JR, TOTAL COUPLE)
   - 3 — STEP3 (GROUP-INDEPENDENT)
2. NUC number of materials to be processed
3. ING number of neutron energy groups ($\leq$100)
4. IGG number of gamma-ray energy groups ($\leq$50)
5. IPO maximum order of scattering anisotropy ($\leq$8)

T Termination of this data block.

2* Neutron energy group boundaries [ING+1] (ING$\neq$0)

The group boundaries are given in the descending order of energy in eV.

3* Gamma-ray energy group boundaries [IGG+1] (IGG$\neq$0)

The group boundaries are given in the descending order of energy in

eV.

T Termination of this data block.

B. First Step (STEP1) Input Instruction (ISTEP=1)

Repeat the input data of STEP1 for each material to be processed.

TITLE CARD Format (12A4)

4$ Integer parameter [4]

1. INALL 0 — only 4$, 5*, and 11* arrays are read
   1 — all input data for this routine are read
2. MATNO ENDF/B tape material number
3. IREW 0 — no effect
   1 — ENDF/B tape is rewound (IREW=1 for first material)
4. NO40 treatment of elastic scattering matrix for thermal group
   0 — no effect
   1 — (ING→ING+1) is added to (ING→ING), where ING is the last group number for neutron groups. SUPERTOG code assumes that the group (ING+1) is the thermal group, but the present system assumes the group ING is the thermal group. Therefore, when SUPERTOG-JR is used as one module of the code system, always NO40 = 1.

5* Resonance information [4]

1. SIGP potential scattering cross section per resonance atom:

$$SIGP = \left(\frac{\Sigma_p}{N} - 4\pi R^2 \right),$$

   where Σ_p is the mixture macroscopic potential cross section, N is the atomic number density of the resonance isotope, and R is the resonance isotope potential scattering length. (SIGP=10^8 for infinite dilution)
2. AJIN input value of J-state for unresolved resonance calculations
3. FRACT r-factor for GAM Nordheim resolved resonance treatment
4. SFACT s-factor for GAM Nordheim resolved resonance treatment

T Termination of this data block

6$ Problem information [18]

1. IDTAP ENDF/B tape identification number
2. MODE 1 — ENDF/B tape is in binary mode
   2 — ENDF/B tape is in BCD mode
3. MCODE output option for GAM code

1 — GAM-1

2 — GAM-II

Note: If MCODE=1, the maximum order of scattering anisotropy is one. Therefore, MCODE=2 must be entered in this code system.

4. IW option for the weighting function

1 — 1/E - function

2 — 1.0

3 — arbitrary weighting function (7$ and 8*)

4 — 1/E joined with a fission spectrum (7*)

5 — exact 1/E

5. N1 0 — no effect

N — number of interpolation regions used for specifying arbitrary weighting function (IW=3)

6. N2 0 — no effect

N — number of points in arbitrary weighting function (IW=3)

7. ISPEC 0 — cross section average calculation

1 — spectrum calculation

8. IRES option for resolved resonance data

0 — only the low energy resolved resonance data are added to the smooth cross section

1 — all resolved resonance data are added to the smooth cross section as infinite dilution cross section

2 — GAM-II output, of which the ℓ=0 resonances are transferred and the ℓ=1 resonance are added to the smooth background

9. IPUN 0 — no punched output

1 — output in the GAM format

2 — output in the ANISN format

3 — output in both the GAM and ANISN formats

4 — punch 1-D cross sections

Note: IPUN = 2 must be entered in this code system.

10. LINK1 0 — no effect

1 — resonance calculation

11. LINK2 0 — no effect

1 — smooth cross section calculation

12. LINK3 0 — no effect

1 — elastic scattering cross section calculation

13. LINK4 0 — not calculate the inelastic scattering matrix

1 — calculate the inelastic scattering matrix from ENDF/B tape
2 — calculate continum part of the inelastic scattering by the Gilbert-Cameron's level density model
3 — calculate continum part of the inelastic scattering by the Newton's level density model

14. LINK5 0 — no effect
1 — calculate (n,2n) scattering matrix

15. LINK6 0 — no effect
1 — calculate displacement cross sections and heat generation coefficients

16. IMUNO 0 — no effect
N — number of the angular mesh points in integral calculation, normally N = 20 (LINK6=1)

17. NEPONT 0 — no effect
N — number of the energy mesh points for one group in integral calculation, normally N = 10 (LINK6=1)

18. NPRINT 0 — no effect
1 — detailed print for each group (LINK6=1)

7* Energy in units of eV, where fission spectrum is jointed with 1/E [1] (IW=4). If the energy does not given, this value is atutomatically set to 6.74 keV.

T Termination of this data block.

7$ Point numbers and interpolation schemes for each interpolation range (NBT(I), JNT(I), I=1, N1) [2*N1] (IW=3)

8* Energies and arbitrary weight functions for each interpolation range (E(I), ϕ(I), I=1, N2) [2*N2] (IW=3)

T Termination of this data block.

11* Data for displacement and heat generation cross section calculation [6] (LINK6=1)

1. ED effective displacement energy (eV)
2. AM atomic weight of the nucleus on ground state
3. AMNG atomic weight of the residual nucleus for (n,γ) reaction
4. AMNP atomic weight of the residual nucleus for (n,p) reaction
5. AMNA atomic weight of the residual nucleus for (n,α) reaction
6. HFB kinetic energy of the fission fragment (eV)

The unit of the atomic weight is ^{12}C=12.0. If the recoil

energy due to the mass difference can be neglected, set AMNG= AMNP=AMNA=0.0

T Termination of this data block.

C. Second Step (STEP2) Input Instruction (ISTEP=2)

TITLE CARD Format (12A4)

4$ Selection of routines [5]

1.	IOPT1	0 — no	THERMOS
		1 — yes	
2.	IPPT3	0 — no	FFACTOR
		1 — yes	
3.	IOPT4	0 — no	POPOP4-JR
		1 — yes	
4.	IOPT5	0 — no	GAMLEG-JR
		1 — yes	
5.	IOPT6	0 — no	TOTAL COUPLE
		1 — yes	

5$ ENDF/B identification numbers of materials to be processed [NUC]

The order of material designation is arbitrary, but it is desirable to select the same order as materials are stored in the library produced by the first step (STEP1).

6$ THERMOS identification numbers of materials to be processed [NUC] (IOPT1=1).

For materials which need not be replaced the last group cross section of SUPERTOG-JR with the thermal group value produced by THERMOS, material identification numbers should be put to zero. The order of material designation must be in the same order as in 5$ array.

The data array from 7$ to 10* should also be in the same order as 5$ array.

7$ JAERI-FAST set identification numbers of materials to be processed (see Appendix D), [NUC] (IOPT3=1)

For a material which is not given in JAERI-FAST set library, identification number is put to zero.

8* Atomic numbers of materials to be processed [NUC] (IOPT5=1)

9* Atomic number densities of materials to be processed [NUC]

10* Temperature (°K) of materials to be processed [NUC]

T Termination of this data block.

C.1 Input instruction for THERMOS (IOPT1=1)

Card 1 Format (I6)

KEY 0 — calculate the thermal cross section by using THERMOS
1 — input the thermal cross section by the card data
If KEY = 0, input the data cards of THERMOS-MUG2 after card 1, but if KEY = 1, repeat the following cards for each material to be processed

Card 2 Format (I6)

MATNO material number defined by 6$ array

Card 3 Format (5E12.5)

σ_a, σ_f, $\nu\sigma_f$, $\sigma_{gg}^{\ell=0}$, $\sigma_{gg}^{\ell=1}$

The order of materials is arbitrary. Put one blank card as an END CARD, when total number of input materials is less than NUC.

C.2 Input instruction for FFACTOR (IOPT3=1)

12$ [2]

1. NGP number of neutron energy groups (25 or 70) of JAERI-Fast set library
2. IPRI 0 — no effect
1 — print the effective microscopic cross section calculated by FFACTOR

T Termination of this data block.

C.3 Input instruction for POPOP4-JR (IOPT4=1)

Repeat the 13$ and 14$ arrays by NUC times for each material to be processed. The order of materials is arbitrary.

13$ [5]

1. MATNO material number defined by 5$ array
2. NMATLS number of reaction types to be treated
3. NFLT number of reaction types to be read from POPOP4 library (NFLT = NMATLS)

4. LOOK 0 — print only the essential results
   1 — print the detailed informations and results
5. MUTT 0 — no effect
   -1 — the gamma-ray production cross sections for all reactions are summed up and the resulting total gamma-ray production cross section is printed (NMATLS≤10)
   1 — same as for MUTT = -1, except the result is also written in a file (NMATLS≤10)
   MUTT should be set to 1 in this code system.

T Termination of this data block.

14$ Identification numbers of reaction types to be read from POPOP4 library (see Appendix E) [NFLT]

T Termination of this data block.

C.4 Input instruction for GAMLEG-JR (IOPT5=1)

17$ [10]

1. IZ number of materials to be calculated (IZ = NUC)
2. N number of integration intervals for each energy group
3. KON -1 — input flux weighting (21* and 22*)
   0 — not weighting
   1 — source weighting (19* and 20*)
4. ICAL 0 — input data for photoelectric, pair production and coherent scattering cross sections by cards (23* and 27*)
   1 — calculate above cross sections and gamma-ray heat generation cross sections in the code.
   When ICAL = 0, the heat generation cross sections are not calculated.
5. IS number of energy points for input source (19* and 20*)
6. IF number of energy points for input flux (21* and 22*)
   If KON = -1, IF = 0.
7. IA number of energy points for input absorption cross sections (23*, 24* and 25*). If ICAL = 1, IA = 0
8. IC number of energy points for input coherent scattering cross sections (26* and 27*).
   If ICAL = 1, IC = 0
9. IPRTO 0 — no effect
   1 — print detailed informations for absorption and coherent

scattering cross sections (ICAL=1)

10. IPRT1 0 — no effect

1 — print detailed informations for heat generation coefficients (ICAL=1)

T Termination of this data block.

19* Energies of input source in the descending order of energy in units of MeV [IS]

20* Input source [IS]

T Termination of this data block.

21* Energies of input flux in the descending order of energy in units of MeV [IF] (KON=-1)

22* Input fluxes [IF] (KON=-1)

T Termination of this data block.

23* Energies at which photoelectric and pair production cross sections are given in the descending order of energy in units of MeV [IA] (ICAL=0)

24* Photoelectric cross sections [IA] (ICAL=0)

25* Pair production cross sections [IA] (ICAL=0)

T Termination of this data block.

26* Energies at which coherent scattering cross sections are given in descending order of energy in units of MeV. [IC] (ICAL=0)

27* Coherent cross sections [IC] (ICAL=0)

T Termination of this data block.

C.5 Input instruction for TOTAL COUPLE (IOPT6=1)

29$ [5]

1. MATID identification number for the region-wise cross section. A same material number is assigned for all Pn components.
2. NPUN output of the cross section table

0 — output to the cross section library

1 — punch cross sections

2 — no effect

3. IPO 0 — print cross sections

1 — no effect

4. NHEAT 0 — no effect

1 — incorporate heat generation coefficient into cross section table

5. NDISP 0 — no effect

1 — incorporate displacement cross section into cross section table

T Termination of this data block.

D. Third Step (STEP 3) Input Instruction (ISTEP=3)

30$ [3]

1. IPG number of groups to be printed
2. NOACT number of activation cross sections, including the heat generation coefficient and displacement cross section
3. ITH type of the cross section table

0 — forward cross section

1 — adjoint cross section

T Termination of this data block

31$ Input-logical-unit numbers of files in which the cross section tabels are stored [NUC]

Note: The numbers should correspond with the numbers assigned with job control macro.

32$ Identification numbers of materials assigned with 29$ array (MATID) [NUC]

Note: The order of the numbers should correspond with the order of the input-logical-unit numbers given in 31$ array.

33$ Group numbers (in the ascending order) to print the cross sections, [IPG] (IPG≠0)

T Termination of this data block.

2.9 Input/Output File Assignment

Input and output files and their logical unit numbers required in each step of the MACS code modules are tabulated in Table 2.9.1, where the abbreviations TCUP and GRPIN are used for TOTAL COUPLE and GROUP-INDEPENDENT, respectively.

Table 2.9.1 Input/output file assignement for MACS

STEP / File	STEP1	STEP2					STEP3
	SUPERTOG	THERMOS	FFACTOR	POPOP4	GAMLEG	TCUP	GRPIN
F01	Scratch			Scratch			Scratch
F02	Scratch	Scratch					Scratch
F03	Scratch						
F04	Scratch						
F08	ENDF/B tape						
F09		THERMOS lib.					
F10				POPOP4 lib.			
F11			Scratch				
F12			effective*3 (n,n)	→	→	→	
F13	Scratch			(n,γ)	→	→	
F14	Scratch				(γ,γ)	→	
F15						Output x-sec →	Input*2 x-sec
F20	Output*1 (n,n) →	→	Input x-sec lib.				
F40							Output lib.
F41			JAERI -Fast set				
F80 ∼ F86	Scratch if LINK6=1						

*1) When many nuclides are processed by STEP1 at one time, the infinite dilution cross section table for the first nuclide is written on the logical-unit of F20, the second on F21, the third on F22, and so on. These files are collected into one file by using TAPE MAKER (see Chap. 4). The collected file is used as an input cross section file for the FFACTOR routine.

*2) Logical unit number for input cross section file is specified by input data 31$ array, so this is not restrained on F15.

*3) The effective cross sections for each nuclide in a homogenized mixture are written in the same form as on the infinite dilution file produced by STEP-1 (see Appendix F).

2.10 Limitation of MACS

The maximum numbers of neutron groups and gamma-ray groups are 100 and 50, respectively, and the maximum number of Legendre expansion terms for the anisotropy of elastic scattering cross sections is 8.

All computational modules are wirtten in the form of flexible array dimension, except SUPERTOT-JR3. A required array size, LIM1, for each module is obtained from the following equations:

a) FFACTOR;

```
LIM1 = 34+9*ING*NUC+8*18*(ING+NSF+NGP)
```

b) TOTAL COUPLE;

```
LIM1 = 15+NOACT*MAXG+ING*(ING+3)*NP+IGG*(IGG+3)*NP
      +ING*IGG+MAX(ING*(ING+3), IGG*(IGG+3), ING*IGG)
      +(NOACT+3+MAXG)*MAXG
```

c) GROUP-INDEPENDENT;

```
LIM1 = 10+2*NUC+IPG+(NOACT+3+MAXG)*MAXG*NP,
```

where ING : number of neutron groups
IGG : number of gamma-ray groups
NP : maximum scattering order plus 1
NOACT : number of activation cross sections
NUC : number of nuclides to be processed
NSF : number of nuclides to be computed the f-factor
NGP : number of neutron groups of JAERI-Fast set library

```
MAXG = ING + IGG,
```

and MAX is a built-in function selecting a maximum value in its arguments.

The value of LIM1 must be greater than any array size required by the above mentioned modules and given in the subroutine SIZE as follows:

```
SUBROUTINE SIZE (LIM1)
COMMON/POP4/D(1), DUMY (80000)
LIM1 = 80000
RETRUN
END
```

The default value of LIM1 is 80000. If this LIM1 is less than the required array size, MACS prints the size needed for the computation and stops the execution.

3. ANISN-JR

Analyses of shield experiments require various quantities such as energy spectra, reaction rates, heat generations, radiation damages, and biological doses. These quantities are obtained by multiplying the fluxes in the shield by response functions of required reactions. The one-deimensional transport calculation code ANISN is widely being used as a standard shielding code, but additional input preparation such as adding the response functions of detectors to the ANISN cross section table are necessary in order to get the above mentioned quantities. These input preparations are, however, somewhat troublesome. In addition, the group cross sections for heterogeneous zone consisting of media of thicknesses of more than several mean free paths have to be averaged by using the flux distribution over the zone as a weighting function.

In order to make these treatments possible and to increase the utility of ANISN, some optional functions are added to the code as follows:

1) print the total fluxes at boundary points,
2) calculate and print the spectrum of $\phi_g/\Delta E_g$ or $\phi_g/\Delta U_g$, where ΔE_g and ΔU_g are respectively the energy and lethargy width of the energy group g,
3) print the angular fluxes at only required meshes,
4) use the asymmetric quadrature set,
5) calculate the reaction rates for neutron and gamma-ray detectors, and collapse the response functions of the detectors,
6) generate volume-flux weighted cross sections for an arbitrary zone or region,
7) collapse into few group cross sections in ANISN, ANISN-JR, MORSE[29] DOT or TWOTRAN[30] format, (In TWOTRAN format, the ℓ-th Legendre coefficient of the scattering cross section is divided by $(2\ell + 1)$ and the cross section of (n, 2n) reaction is added for use of the coarse mesh rebalance technique)
8) multiply the averaged cross section by the density factor, when an option of density factors are used (IDFM = 1).
9) plot the flux distribution, the energy spectrum and/or reaction rate distribution by using the ANISN-PLOT written as a utility code of ANISN-JR.

Note) In both ANISN and ANISN-JR, the adjoint calculation can not be performed with the group independent cross section tape (ID2 = 1)

but with the tape generated from step 3 (ITH = 1) of the MACS code modules.

The ANISN code with the above mentioned new options is named as ANISN-JR.[13] The input instruction as well as the program list of ANISN-PLOT are shown in Ref. 13).

3.1 Input Instruction for ANISN-JR

The free-form FIDO format shown in Appendix A is used for preparing input data for ANISN-JR. To select the free-form, an array is identified as a ** or a $$ depending on whether it is floating or integer array. In the following, the array dimension is given in square blackets, and the condition under which the array is to be specified is given in parentheses. The array without the condition should always be specified.

A. Parameters for ANISN-JR

A - 1 Format (2I5)

1. IANISN — the format of group independent cross section tape.
   0 — same as the original format
   1 — for the tape produced by RADHEAT-V3
2. ITMAX — maximum execution time in minutes. If ITMAX = 0, this option is ignored.
   ANISN checks this time at the end of each outer iteration and, if it has been exceeded, the problem is terminated with full output.

A - 2 Format (11I5)

1. IIBOUND
   0 — print total fluxes at midpoints of each mesh interval (same as original)
   1 — print total fluxes at boundaries of each mesh interval
2. IISPTM
   0 — no effect
   1 — calculated and print neutron spectra $\phi_g/\Delta E_g$ at each mesh
   2 — calculate and print neutron spectra $\phi_g/\Delta U_g$ at each mesh
   Energy group boundaries are specified by cards B.
3. IIANLL
   0 — print angular fluxes at all space meshes (same as original)

1 — print angular fluxes at only required meshes
The required space meshes are given by cards C. If angular fluxes are required, ID1 = 1 must be entered in 15$ array.

4. IGMNEW — number of total energy groups (equal to IGM in 15$ array)

5. IGMNEU — number of neutron groups.
If neutron or gamma-ray only, IGMNEU = IBMNEW.

6. NACTPR
0 — no effect
1 — print activities for each group and zone

7. NREACT
0 — no effect
1 — calculate and print reaction rates for neutrons and gamma rays
2 — calculate reaction rates and also collapse response functions of detectors in region wise
3 — collapse in region wise response functions and punch of detectors
The response functions for neutrons and gamma rays are given by cards K.
For collapsing the response functions, IFG = 1 in 15$ array, and 27$, 28$ and 29$ arrays must be entered.

8. NASYMM
0 — no effect
1 — use asymmetric quadrature set
The angular quadrature weights and cosines are given by 6* and 7* arrays. In the case NASYMM = 1, the reflective condition for left boundary cannot be used.

9. NRESAT
0 — no effect
1 — write/read final fluxes on a tape for use as an initial flux guess for the next run
Final fluxes are written on the logical unit No. 15 and read from No. 14. For the first run, NRESAT = 1 and IFN = 1 or 2 in 15$ array must be specified, and for the following, NRESAT = 1 and IFN = 3.

10. NXSOUT
0 — no effect
1 — obtain the few group cross sections for ANISN-JR, DOT, TWOTRAN or MORSE (IFG = 1 in 15$, and 27$,

28$ and 29$ arrays)

When NXSOUT = 1, cards D are necessary.

11. NPLOT — 0 — no effect

1 — obtain the file for plotting

B. Energy group boundaries (IISPTM = 1 and NPLOT = 1)

B - 1 Format (I5)

1. NOYGRE — number of energies to be specified in the next cards

NOYGRE = IGM + 1, for neutron or gamma-ray problems

NOYGRE = IGM + 2, for coupled neutron and gamma-ray problems

B - 2 Format (8E10.5)

(YGRENE(I), I = 1, NOYGRE)

Energy group boundaries are given in the descending order of energy in eV

C. Meshes to print angular fluxes (IIANLL = 1)

C - 1 Format (I5)

1. NOANNO — number of meshes to print angular fluxes ($\leq$10)

C - 2 Format (10I5)

(NOANLL(I), I = 1, NOANNO)

meshe numbers to print angular fluxes

D. Parameters for collapsing (NXSOUT = 1)

D - 1 Format (6I5)

1. NACT — number of cross sections for activation calculations to be added to the top of the cross section table

2. IDOT — 0 — calculate collapsed cross sections in TWOTRAN format

1 — calculate collapsed cross sections in DOT (or ANISN-JR) format

3. NPU — output of cross section tables

0 — only print

1 — punch

2 — write on a tape (logical unit No. 40)*
3 — add cross sections to the tape produced in previous cases.*

4. IGNT — number of groups of (n, 2n) down-scattering
Normally, total number of neutron groups is entered.
When IDOT = 1 (DOT format), IGNT is put to zero.

5. IGMN — number of energy groups to be obtained from collapsed groups (from highest energy).

6. ITL2 — length of the output cross section table
Specify ITL2 = NACT + IGMN + 3 for DOT and ANISN-JR, and ITL2 = NACT + IGMN + 5 for TWOTRAN.

E. Title of the problem

E - 1 Format (18A4)
(TITLE (I), I = 1, 18)

F. Parameters for ANISN

15$ Integer parameters [36]

1. ID — problem ID number
2. ITH — 0 — forward solution
1 — adjoint solution
3. ISCT — maximum order of scattering found in any zone
4. ISN — order of angular quadrature
5. IGE — 1 — slab; 2 - cylinder; 3 — sphere
6. IBL — left boundary condition
0 — vacuum (no reflection)
1 — reflection
2 — periodic
3 — white/albedo
7. IBR — right boundary condition with the same options as for IBL
8. IZM — number of zones or regions
9. IM — number of mesh intervals
10. IEVT — eigenvalue type
0 — fixed source
1 — k calculations

* Output form on a tape is the same as that of region-wise cross sections produced by MACS STEP-2, so TAPE MAKER can handle this tape.

27.	ID3	0 — no effect N — compute N activities by zone where N is any positive integer
28.	ID4	0 — no effect 1 — compute N activities by interval where N refers to ID3
29.	ICM	maximum number of outer iterations
30.	IDAT1	0 — all data in core storage 1 — store cross sections and fixed sources on tape 2 — fluxes and currents on tape also
31.	IDAT2	0 — no effect 1 — execute diffusion solution for specified groups (24$)
32.	IFG	0 — no effect 1 — obtain flux weight cross sections (27$ and 28$)
33.	IFLU	0 — use step model when linear extrapolation yields negative flux (mixed mode) 1 — use linear model only 2 — use step model only
34.	IFN	0 — enter fission guess (2*) 1 — enter flux guess (3*) 2 — use fluxes from previous case 3 — use fluxes from restart tape
35.	IPRT	0 — print cross sections 1 — do not print cross sections
36.	IXTR	0 — calculate P_L scattering constants (Legendre coefficients) 1 — read P_L constants from cards (34*)

16* Floating point parameters [14]

1.	EV	first guess for eigenvalue
2.	EVM	eigenvalue modifier
3.	EPS	desired accuracy (epsilon)
4.	BF	buckling factor (normally 1.420892)
5.	DY	cylinder or plane height for buckling correction
6.	DZ	plane depth for buckling correction
7.	DFM1	transverse dimension for void streaming correction
8.	XNF	normalization factor
9.	PV	0.0, k_0, or α_0 according to IPVT = 0, 1, or 2

2 — α calculations
3 — concentration search
4 — zone width search
5 — outer radius search
6 — buckling search

11. IGM — number of energy groups
12. IHT — position of σ_t in cross section table
13. IHS — position of σ_{gg} in cross section table
14. IHM — length of cross section table
15. MS — cross section mixing table length (10$, 11$ and 12*)
16. MCR — number of cross section sets to be read from cards (14*)
17. MTP — number of cross section sets to be read from tape (13$)
18. MT — total number of cross section sets (elements + mixtures)
19. IDFM
    0 — no effect
    1 — use density factors (21*)
20. IPVT
    0 — no effect
    1 — enter k_0 as PV (16*)
    2 — enter α_0 as PV
21. IQM
    0 — no effect
    1 — enter distributed source (17*)
22. IPM
    0 — no effect
    1 — enter shell source by group and angle (18*)
    IM — enter shell source by interval, group, and angle
23. IPP — interval number which contains shell source if IMP = 1; 0 otherwise
24. IIM — maximum number of inner iteration
25. ID1
    0 — no effect
    1 — print angular fluxes
    2 — punch scalar fluxes
    3 — both 1 and 2
26. ID2
    0 — no effect
    1 — use specially prepared group independent cross section tape (contains MTP materials)
    2 — use cross sections and fixed source from previous problem

10. RYF — λ_2 relaxation factor (normally 0.5)
11. XLAL — point flux convergence criterion if entered greater than zero
12. XLAH — upper limit for $|1.0 - \lambda_1|$ used in linear search
13. EQL — eigenvalue change epsilon
14. XNPM — new parameter modifier

Note: The above data block is followed by a T.

G. Cross sections {ID2 = 0}

13$ Library ID numbers [MTP] {MTP > 0}

14* Cross sections [MCR × IGM × IHM] {MCR > 0}

Note: If entered, the above data block is followed by a T.

H. Fixed source {IEVT = 0 and ID2 < 2}

17* Distributed source [IGM × IM] {IQM = 1}

18* Shell source [IGM × IPM × MM] {IPM > 0}

Note: If entered, the above data block is followed by a T.

I. Flux or fission guess {IFN < 2}

2* Fission density [IM] {IFN = 0}

3* Flux guess [IGM × IM] {IFN = 1}

Note: If entered, the above data block is followed by a T.

J. Remainder of data

1* Fission spectrum [IGM]

4* Radii by interval boundary [IM + 1]

5* Velocities [IGM]

6* Angular quadrature weights [MM][a)]

7* Angular quadrature cosines [MM]

8$ Zone numbers by interval [IM]

9$ Material numbers by zone [IZM]

10$ Mixture numbers in mixing table [MS] {MS > 0}

11$ Component numbers in mixing table [MS] {MS > 0}

12* Number densities in mixing table [MS] {MS > 0}

19$ Order of scattering by zone [IZM] {ISCT > 0}

20* Radius modifiers by zone [IZM] {IEVT = 4}

---

a) MM = ISN + 1 for plane or sphere, (ISN × (ISN + 4))/4 for cylinder

21* Density factors by interval [IM] {IDFM = 1}

22$ Material numbers for activities [ID3] {ID3 > 0}

23$ Cross section table position for activities [ID3] {ID3 > 0}

24$ Diffusion calculation markers [IGM] {IDAT2 = 1}

25* Albedo by group at right boundary [IGM] {IBR = 3}

26* Albedo by group at left boundary [IGM] {IBL = 3}

27$ Few group parameters [5] {IFG = 1}

1. ICON
   - 0 — no effect
   - 1 — microscopic cross sections desired
   - 2 — macroscopic cross sections desired (minus implies cell weighting)
   - 3 — macroscopic cross section desired (cell weighted for arbitrary zones (29$)
2. IHTF — position of σ_t in weighted cross sections
3. IHSF — position of σ_{gg} in weighted cross sections (minus implies up-scattering removal)
4. IHMF — table length of weighted cross sections
5. IPUN
   - 0 — no effect
   - 1 — punch weighted cross sections
   - 2 — obtain weighted cross sections tape F11.[a)]

28$ Few group number for each multigroup [IGM] (IFG = 1)

29$ Cell number for each zone.
This number becomes material number for cell weighted cross sections [IZM] (IFG = 1 and ICON = 3)

34* P_L scattering constants [JT × MM][b)] (IXTR = 1)

Note: The above data block is followed by a T.

K. Detector responses (NREACT = 0)

(When the neutron and gamma-ray responses are required, the responses of detectors must be given respectively, that is, at first the neutron's data and then the gamma-ray's data)

---

a) Output format is the same as that of region-wise cross sections generated by MACS STEP-2, so TAPE MAKER can handle this tape.

b) JT = ISCT for plane or sphere, (ISCT × (ISCT + 4))/4 for cylinder

Note: JT is truncated to the next lower integer for cylinders when ISCT is odd.

K - 1 Format (I5)

1. NELM number of detectors for which the response functions for neutrons or gamma rays are given

K - 2 Format (I5, 4A4)

1. NAME identification number for the detector
2. DXCM title of the detector

K-3 Format (8E10.5)

(OSIG(I), I = 1, NG)

responses of the detector are given in the descending order of energy, where NG is the number of neutron or gamma-ray groups. (Cards K-2 and K-3 are repeated by NELM times)

In ANISN-JR module, for any selection of parameters for IIBOUD and IISPTM, the collapsed cross sections and the detector responses are obtained by using the flux at midpoint of mesh intervals as a weighting function.

3.2 Input/Output File Assignment

ANISN-JR requires the input/output files shown in Table 3.1 during the execution. ANISN-JR can generate the volume-flux weighted cross section for an arbitrary zone or region as given in Table 3.2. The first column gives types of weighted cross sections and input options, and the second shows the input data array for collapsed group structure desired. The third, fourth and fifth columns show the zone, in which the cross sections are collapsed, number of cross section sets to be output and logical unit number of output file, respectively.

3.3 Limitations for ANISN-JR

ANISN-JR adopts a flexible dimensioning technique, however, at the execution of a problem, the maximum number of locations available for ANISN data, LIM1, must be specified in the main program as follows:

```
CCC     ANISN-JR MAIN PROGRAM
        COMMON/BULKBU/D(1), LIM1, DUMY(×××××)
C       SET BLANK COMMON SIZE
        LIM1 = ×××××
        CALL ANISN
```

```
      STOP
      END
```

The present code assignes LIM1 = 50,000 as a default value. The restrictions for ANISN-JR are as follows:

(1) For options of IIBOUD = 1 (print total flux at the boundary point) and IISPTM = 1 (print spectrum), IDATI $\neq$ 2 (fluxes in core) must be entered in 15$ array.
Dimensional limitation: IGM × (IM + 1) $\leq$ 30000.

(2) For option of IIANLL = 1 (print anguler fluxes), the maximum number of intervals to be printed is 10.

(3) Detailed print of activities.
Dimensional limitation: IGM × ID3 × (IM = IZM + 1) $\leq$ 30000, where ID3 is the number of activities in 15$ array.

(4) For calculations of reaction rates, the maximum number of detectors, energy groups and mesh intervals are respectively 25, 100 and 400.

(5) Output of the weighted cross sections in DOT, ANISN-JR or TWOTRAN format.
Dimensional limitation: (IHMF + ITL2) × IGMF $\leq$ 1040.

Table 3.1 Input/output file assignment for ANISN-JR

Logical unit No.	Comment
F01	Scratch file
F02	Scratch file (use if IDAT1=1 or 2)
F03	Scratch file (use if IDAT1=2)
F04	Library tape
F05	Input
F06	Print output
F08	Scratch file (use if IDAT1=2)
F09	Scratch file (use if NXSOUT=1)
F11	Output of the weighted cross section (use if IPUN=2)
F14	Input of the restart file (use if NRESAT=1)
F15	Output of the restart file (use if NRESAT=1)
F20	Scratch file (use if IIBOUND=1)
F30	Output of the plotting data (use if NPLOT=1)
F40	Output of the DOT or TWOTRAN cross sections (use if NXSOUT=1 and NPU=2 or 3)

Table 3.2 Types of weighted cross sections and input options

Form of Xsec[1]	Group structure	Region	Number of Xsec sets to be output	Logical unit No.
Micro. Xsec (ICON=1)	28$ array	Each zone	$\sum_{I=1}^{IZM} MS(I)^{2)} \times (ISCT+1)$	F11
Macro. Xsec (ICON=2)	28$ array	Each zone	IZM×(ISCT+1)	F11
Cell weighted Xsec (ICON=-2)	28$ array	Each zone[3]	IZM×(ISCT+1)	F11
Cell weighted Xsec (ICON=3)	28$ array	29$ array	(Number of cell in 29$ array)×(ISCT+1)	F11
Few group Xsec for 2-D codes (NXOUT=1)	Format conversion of the collapsed Xsec in above cases			F40
Collapsed response functions (NREACT≥2)	28$ array	Each zone	IZM×NELM[4]	Cards output

1) Xsec means cross sections.

2) MS(I): number of elements assigned for the I-th zone.

3) Cross sections for each zone produced by this option are weighted values normalized by total flux integrated over all zones. Therefore, these cross section sets must be summed up over each zone to get the cell weighted cross section.

4) NELM: number of neutron detectors + number of gamma-ray detectors .

4. TAPE MAKER

TAPE MAKER is a utility module for editing and updating the files of the cross sections generated by RADHEAT-V3, and can deal with the files produced by STEP-1 (infinite dilution cross sections), and STEP-2 and ANISN-JR (coupled neutron and gamma-ray cross sections). The capabilities of the module are as follows;

1) put together the cross section tables of many nuclides or materials into one file,
2) edit a new cross section file by gathering nuclides according to the requests of users,
3) update the identification name and/or number and the cross section values of any energy groups for any nuclides or materials selected by users,
4) convert a cross section file from binary mode to BCD mode, or vice versa, and
5) print and/or plot the cross sections of any reactions or materials selected by users.

Nuclides and materials mentioned above mean the nuclides with the infinite dilution microscopic cross sections and the materials with the macroscopic cross sections, respectively. The reaction types which can be updated, printed and plotted from cross section tables are shown in Table 4.1. The forms of cross section file are shown in Appendix F.

4.1 Input Instruction

(1) CARD 1 Format (12A4)

Title card

(2) CARD 2 Format (10I6)

1. ISTEP selection of the cross section file to be handled
   1 — infinite dilution cross section file
   2 — coupled neutron and gamma-ray cross section file
2. NUC number of materials to be handled. If NUC is zero, the cross section file is duplicated on a backup file.
3. ING number of neutron energy groups
4. IGG number of gamma-ray energy groups
5. LORDER maximum order of scattering anisotropy

6. NOACT number of activation cross sections
7. NPRINT number of reaction types to be printed
8. NPLOT number of reaction types to be plotted
9. ITYPE 0 — input tape is in binary mode
   N — input tape is in BCD mode
   N indicates the logical unit number of the input tape
10. JTYPE 0 — output tape is in binary mode
    N — output tape is in BCD mode
    N indicates the logical unit number of the output tape.

(3) CARD 3 Format (6E12.5)
(ERGRP(N), N=1, ING+1) (NPLOT≠0, ISTEP=2)
Neutron energy group boundaries. The group boundaries are given in the descending order of energy in eV.

(4) CARD 4 Format (A8)
(NPRT(N), N=1, NPRINT) (NPRINT≠0)
The names of the reaction types to be printed (see Table 4.1). One name is given in one card.

(5) CARD 5 Format (A8)
(NPLT(N), N=1, NPLOT) (NPLOT≠0)
The names of the reaction types to be plotted. (see Table 4.1) One name is given in one card.

The next CARD 6 and CARD 7 are repeated by NUC times. If NUC = 0, omit CARD 6 and CARD 7, and when NUPDT = 0, omit CARD 7.

(6) CARD 6 Format (5I6, 12A4)
1. NUNIT The logical unit number of tape where the cross section tables are stored
2. MATNO material number to be handled
3. IREW 0 — not rewind the tape
   1 — rewind the tape
4. NUPDT number of cross section data to be updated
5. NWMAT new material identification number, if it is necessary to change MATNO. If NWMAT = 0, MATNO is regarded as the name of new material.
6. NWCM new title for the new material. When NWMAT ≠ 0, the old

title is replaced by this title.

(7) CARDS 7 Format (A8, I6, E16.5)

Data for cross sections to be updated. One set of data is given in one card. The order of the data is arbitrary.

1. NREACT identification name of the reaction type to be updated (see Table 4.1)
2. NGRP group number of the cross section to be updated
3. CROSS value of the cross section to be updated

4.2 Input/Output File Assignment

TAPE MAKER requires the following input/output files.

Input files : logical units containing group cross sections for NUC materials. The numbers of each logical unit must be specified on CARD 6 (NUC ≠ 0).
When NUC = 0 and ITYPE = 0, F01 unit is used as an input unit for binary mode library, and ITYPE=N (N>0), the logical unit number N is used as an input unit for BCD mode library.

Output files : F40 except NUC=0 and ITYPE=N (N>0).
When NUC=0 and JTYPE=N, the logical unit number N is used as the output unit for BCD mode library.

Note : ITYPE and JTYPE on CARD 2 are normally set to zero. These options are only available when NUC is put to zero.

Table 4.1 Identification names of reaction types which can be printed, plotted and updated

No.	Identification names	Option and steps						Comments
		PRINT		PLOT		UPDATE		
		1st	2nd	1st	2nd	1st	2nd	
1	TOTAL			○1)	○	*2)	○	total
2	CAPTURE			○		*		capture
3	FISSION			○		○		fission
4	NU			○		○		neutrons per fission
5	(N,P)			○		○		(n,p) reaction
6	(N,A)			○		○		(n,α) reaction
7	(N,G)			○		○		(n,γ) reaction
8	ELAS			○		*		total elastic scattering
9	INELAS			○				total inelastic scattering
10	(N,2N)			○				total (n,2n) reaction
11	SMOOTH	○		○				include the reactions from No.1 to 10
12	ABSORB			○	○	*	○	absorption
13	NU*FIS			○	○	*	○	$\nu\sigma_f$
14	SIGS(P0)					○	○	P_0 component of self-scattering
15	SIGS(P1)					○	○	P_1 component of self-scattering
16	SCATTER	○	○3)					scattering transfer matrix
17	HEAT	○		○	○			heat generation coefficient
18	DISPLACE	○		○	○			displacement cross section

1) The sign of circle, ○ , shows the reaction types which can be updated, printed and plotted from the cross section tables.

2) The sign of star, *, shows that the cross sections are recalculated so as to maintain the balance between reaction cross sections, when cross sections for any reaction types are updated.

3) It is printed that all reaction types including the cross section table shown in Table 2.6.1.

5. Sample Problems

This chapter desribes input data for three sample problems which generate infinite dilution cross sections, region-wise neutron and gamma-ray coupled cross sections for a homogenized mixture and for heterogenous cells, and a sample problem which edits and updates the cross section library by using TAPE MAKER.

In these sample problems, numbers of neutron and gamma-ray groups are 26 and 8, respectively. Scattering matrices are in the P_3 approximation.

5.1 Sample Problem No.1 - Production of Infinite Dilution Cross Sections and Library.

Infinite dilution cross sections for carbon and iron are calculated in MACS step 1 and are combined to an infinite dilution library by TAPE MAKER. The displacement cross sections and the heat generation are also calculated. Basic neutron cross sections for iron (MAT=1192) and carbon (MAT=1274) are taken from ENDF/B-IV libraries.

When an infinite dilution library is produced by using TAPE MAKER, the thermal group cross sections obtained in the step 1 of MACS are replaced by the data for a Maxwellian distribution. The flow diagram of the sample problem calculation is shown in Fig. 5.1 and input data set for each step is given in Tables 5.1.1 ∿ 5.1.3, respectively.

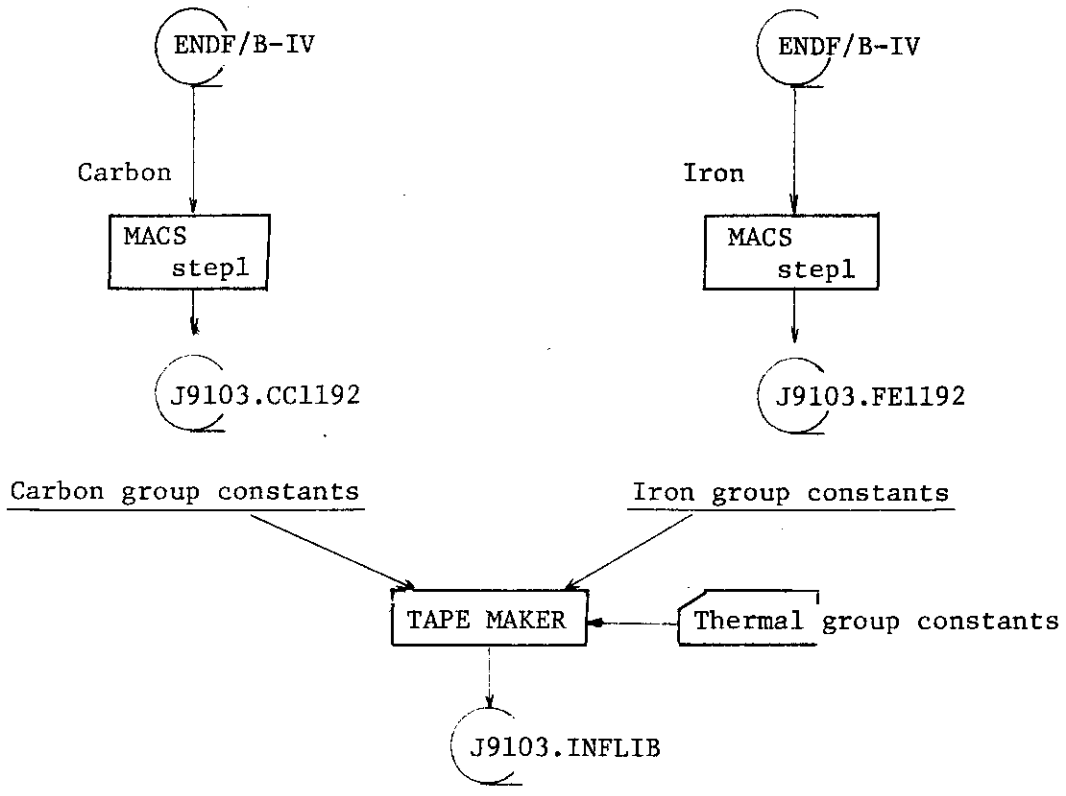

Fig. 5.1 Calculational flow of the sample problem No.1 to produce an infinite dilution library

Table 5.1.1 Input data of the sample problem No.1 to generate infinite dilution cross sections for carbon by using the step 1 of MACS

```
*HRUN   EFNAME=J9103.RADHEAT3
*DISK F01
*DISK F02
*DISK F03
*DISK F04
*TAPE   F08,J1615.ENDFB4.OLD,001575
*DISK F13
*DISK F14
*DISKTN F20,J9103.FE1192,TRK=20
*DISK F80
*DISK F81
*DISK F82
*DISK F83
*DISK F84
*DISK F85
*DISK F86
*DATA
 1** 1 1 26 0 3 T
 2** 1.5+7 1.05+7 6.5+6 4.0+6 2.5+6 1.4+6 8.0+5 4.0+5 2.0+5 1.0+5
     4.65+4 2.15+4 1.00+4 4.65+3 2.15+3 1.00+3 4.65+2 2.15+2 1.00+2
     4.65+1 2.15+1 1.00+1 4.65 2.15 1.00 4.65-1 1.0-3
  T
     FE   1192  ENDF/B-IV
 4** 1  1192  1  1
 5**   1.0+8 10.0   0.0   0.0 T
 6** 1  2  2  4  0  0  0  1  2  1  1  1  1  1  1  20  10  0
 7**   4.0+5 T
11**  33.0  55.93493  56.93539  55.93891  52.94065  0.0  T
```

Table 5.1.2 Input data of the sample problem No.1 to generate infinite dilution cross sections for iron by using the step 1 of MACS

```
*HRUN    EFNAME=J9103,RADHEAT3
*DISK F01
*DISK F02
*DISK F03
*DISK F04
*TAPE    F08,J1615.ENDFB4,OLD,001575
*DISK F13
*DISK F14
*DISKTN F20,J9103,FE1192,TRK=20
*DISK F80
*DISK F81
*DISK F82
*DISK F83
*DISK F84
*DISK F85
*DISK F86
*DATA
 1** 1 1 26 0 3 T
 2** 1.5+7 1.05+7 6.5+6 4.0+6 2.5+6 1.4+6 8.0+5 4.0+5 2.0+5 1.0+5
     4.65+4 2.15+4 1.00+4 4.65+3 2.15+3 1.00+3 4.65+2 2.15+2 1.00+2
     4.65+1 2.15+1 1.00+1 4.65 2.15 1.00 4.65-1 1.0-3
  T
     FE   1192  ENDF/B-IV
 4** 1  1192  1  1
 5**   1.0+8 10.0   0.0   0.0 T
 6** 1  2  2  4  0  0  0  1  2  1  1  1  1  1  1  20  10  0
 7**   4.0+5 T
11**  33.0  55.93493  56.93539  55.93891  52.94065  0.0  T
```

Table 5.1.3 Input data of the sample problem No.1 to produce an infinite dilution library by using TAPE MAKER

```
*MLIEDRUN  RUNNAME=J9103,TAPEMAKE,CLIFD=CLIED,GAFD=ON,COMLIB=CALL
*DISKTO    F01,J9103,CC1274
*DISKTO    F02,J9103,FE1192
*DISKTN    F40,J9103,INFLIB,TRK=20
*DISK      F41
*GCOM35
*DATA
   INFINITE DILUTION LIBRARY ( N=26, P=3 )
     1      2     26      0      3      0      1      1      0      0
SMOOTH
TOTAL
      1  1274       1      2
(N,G)          26  0.00301
SIGS(P0)       26  5.5740
      2  1192       1      2
(N,G)          26  2.2300
SIGS(P0)       26  12.293
```

5.2 Sample Problem No.2 - Production of Region-Wise Coupled Neutron and Gamma-Ray Cross Sections in a Homogenized Mixture.

This problem calculates the neutron and gamma-ray flux distributions in a homogenized mixture composed of carbon and iron by using ANISN-JR, and generates a few group cross sections for two-dimensional code, TWOTRAN, using the above flux distributions as a weighting function.

At the first step, coupled neutron and gamma-ray cross sections of the homogenized mixture are calculated from the infinite dilution cross sections for carbon and iron produced by the sample problem No.1. by using the step 2 of MACS.

In the next step, the neutron and gamma-ray distributions in the shield shown in Fig. 5.2.1 are calculated to generate the few group cross sections by using ANISN-JR.

A homogenized mixture of carbon and iron is 60 cm thick and devided into five zones. Atomic densities of carbon (ENDF/B-IV, MAT=1274) and iron (MAT=1192) in the mixture are 1.3855×10^{22} and 7.9837×10^{22} atoms/cm^3, respectively. The region-wise few group cross sections are required for each zone. In the ANISN-JR shield calculation, a fixed source is distributed in the zone 1 with a density factor of 0.7. The source energy, fine and few group structure are given in the sample input data lists, Tables5.2.1 and 5.2.2.

The calculational flow for the sample problem No.2 is shown in Fig. 5.2.2.

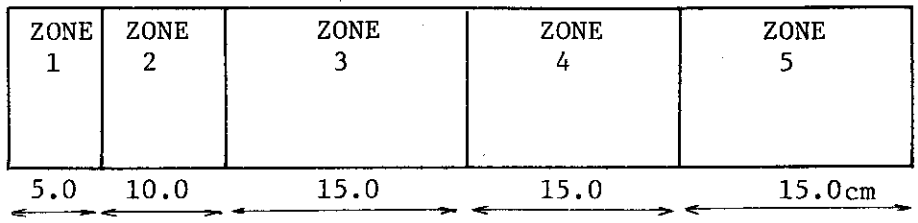

Fig. 5.2.1 One dimensional calculational geometry of the sample problem No.2. Shield materials of each zone are 9 homogenized mixture of carbon and iron. The fixed source is distributed in zone 1 with the density factor of 0.7.

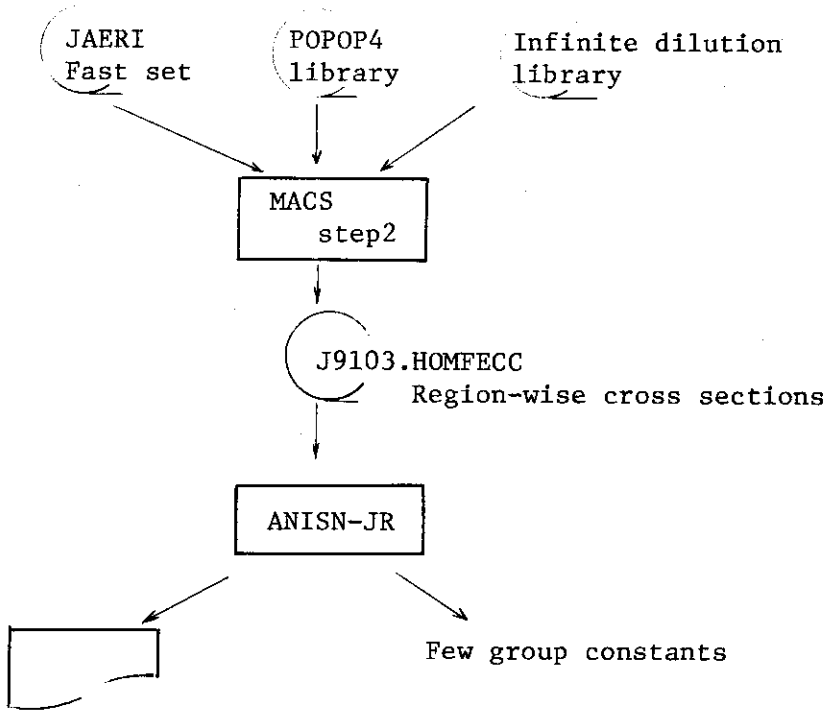

Fig. 5.2.2 Calculational flow of the sample problem No.2

Table 5.2.1 Input data of the sample problem No.2 for the generation of region-wise cross sections by using the step 2 of MACS

```
*HRUN  EFNAME=J9103,RADHEAT3,SIZE=20
*DISK      F01
*DISKTO    F10,J9103.POPBIN2
*DISK      F11
*DISK      F12
*DISK      F13
*DISK      F14
*DISKTN    F15,J9103.HOMFECC
*DISKTO    F20,J9103.INFLIB
*DISKTO    F41,J9103.JFSET25
*DATA
 1**  2  2  26  8  3  T
 2** 1.5+7 1.05+7 6.5+6 4.0+6 2.5+6 1.4+6 8.0+5 4.0+5 2.0+5 1.0+5
     4.65+4 2.15+4 1.00+4 4.65+3 2.15+3 1.00+3 4.65+2 2.15+2 1.00+2
     4.65+1 2.15+1 1.00+1 4.65  2.15  1.00  4.65-1 1.00-3
 3** 10.2+6 8.0+6 6.0+6 4.0+6 2.5+6 1.2+6 5.0+5 1.0+5 1.0+4
  T
  HOMOGENIOUS REGION ( CARBON AND IRON )
 4**  0  1  1  1  1
 5**  1274  1192
 7**     6    26
 8**     6.0  26.0
 9**  1.3855-2  7.9837-2
10**   300.0 300.0
  T
12**  25  0  T
13**  1274  2  2  0  1  T
14**  60102  60304  T
13**  1192  2  2  0  1  T
14**  266301  269102  T
17**  2  10  0  1  9  5R0  T
19**  10.2 8.0 6.0 4.0 2.5 1.2 0.5 0.1 0.01
20**  F1.0  T
29**  10  0  0  1  1  T
```

Table 5.2.2 Input data of the sample problem No.2 for the generation of few group constants for TWOTRAN by using ANISN-JR

```
#HFORT
      COMMON /BULKBU/D(1),LIM1,DUM( 40000)
      LIM1= 40000
      CALL ANISN
      STOP
      END
#HLIED RENAME=J9103.ANISNJR,EDIT=YES,B=NOMAP
SGMT  ANSMS
SELECT (FIMAIN,CLEAR,CONTRL,ERRO,WOT,SPIE,ITIME,CLOCK,ADDR,ANISN)
SGMT  ANS01,CHN=ANSMS
SELECT (PLSNT,FIDO,TP,ADJNT,S804,S805,S814,WOT8,S966,FFREAD)
SGMT  ANS02,CHN=ANSMS
SELECT (GUTS,S807,S810,S821,S824,S833,DT,CELL,S851)
SGMT  ANS03,CHN=ANSMS
SELECT (FINPR,FINPR1,PUNSH,DTFPUN,FLTFX,NWSUB1,NWSUB2,ERRMSG,ACTPRT,    /
      WOTYT)
SGMT  ANS04,CHN=ANS03
SELECT (BT,SUMARY,FACTOR,NWSUB3,NWSUB4)
SGMT  ANS05,CHN=ANS03
SELECT (FEWG,WATE,CONVT,CRATE)
FIN
#HRUN SIZE=20
#DISK       F01
#DISK       F02
#DISKTO     F04,J9103,HOMFECC
#DISK       F09
#DISKTN     F10,J9103,RFLUX,TRK=20
#DISKTN     F40,J9103,TWOXSEC
#DATA
    1    0
    0    2    1   34   26    0    2    0    1    1    0
   36
 1.50E+07  1.05E+07  6.50E+06  4.00E+06  2.50E+06  1.40E+06  8.00E+05  4.00E+05
 2.00E+05  1.00E+05  4.65E+04  2.15E+04  1.00E+04  4.65E+03  2.15E+03  1.00E+03
 4.65E+02  2.15E+02  1.00E+02  4.65E+01  2.15E+01  1.00E+01  4.65      2.15
 1.0       4.65E-01  1.00E-03  1.00E+07  8.00E+06  6.00E+06  4.00E+06  2.50E+06
 1.20E+06  5.00E+05  1.00E+05  1.00E+04
    4
    7   22   37   52
    2    0    2    6   11   18
 SAMPLE INPUT FOR A HOMOGENIOUS SHIELDING
15**  100  0  3  4  1  1  0  5 60  0 34  5  6 39  0  0  4  4  1  0  1  0
        0 40  1  0  0  0  1  1  0  1  0  1  1  0
16**  1.05  0.01  1.0-4  1.421  0.0  0.0  0.0  1.0  0.0  0.5  5.0-4
      0.01  0.0   0.0
 T
13**  4R10  T
17**
 5R9.5824-4 55R0.0 5R1.6925-2 55R0.0 5R8.4287-2 55R0.0 5R1.7297-1 55R0.0
 5R2.6260-1 55R0.0 5R2.0558-1 55R0.0 5R1.4845-1 55R0.0 5R6.6319-2 55R0.0
 5R2.6377-2 55R0.0 5R1.0467-2 55R0.0 5R3.4358-3 55R0.0 5R1.0915-3 55R0.0
 5R3.4860-4 55R0.0 5R1.1132-4 55R0.0 5R3.4905-5 55R0.0 5R1.1081-5 55R0.0
 5R3.5287-6 55R0.0 5R1.1050-6 55R0.0 5R3.5064-7 55R0.0 5R1.1161-7 55R0.0
 F0.0  T
 3**  F0.0  T
```

Table 5.2.2 (continued)

```
 1**  F0,0
 4**  5910,0  60,0
 5**  F1,0
 6**   0.0          0,1666667   0,3333333   0,3333333   0,1666667
 7**  -0,9367418  -0,8688903  -0,3500212   0,3500212   0,8688903
 8**  5R1  10R2  15R3  15R4  15R5
 9**  5R1
19**  5R3
21**  5R0.7  55R1.0
27**  2  5  6  16  0
28**  2R1  3R2  4R3  6R4  6R5  2R6  2R7  8  3R9  3R10  2R11
  T
   3
  18Fe56(N,P)
9.5169-02 3.8483-02 3.3460-03 6.9253-07


  13IN115(N,N')
.11900     .20010     .25375     .33875     .26385     .62811-1   .9033-2    .14634-3


  20DOSE MREN/HR/FLX
1.50-01    1.50-01    1.50-01    1.36-01    1.25-01    1,36-01    25-01      8,30-02
4.20-02    3.00-02    1.80-02    1.00-02    5.90-03    4,40-03    40-03      4,40-03
4.40-03    4.40-03    4.40-03    4.40-03    4.40-03    4.40-03    40-03      4,40-03
4.40-03    3,75-03
  1
  1GAMMA MR/HR/FLX
9.80-03    8.10-03    6.30-03    4.60-03    3.00-03    1.55-03    20-04      8.00-04
```

5.3 Sample Problem No.3 - Production of Region-Wise Coupled Neutron and Gamma-Ray Cross Sections in Heterogeneous Cells

This problem calculates the neutron and gamma-ray fluxes in heterogeneous cells and generates volume-flux weighted cross sections for each region. At first, the coupled neutron and gamma-ray cross sections for the carbon or iron region are calculated in the step 2 of MACS. Secondly, a group-independent tape is produced from the region-wise cross section files in the step of MACS. Then finally, region-wise cross sections averaged over heterogeneous regions are produced by ANISN-JR. The geometry used for the present sample problem is shown in Fig. 5.3.1. The zones 1, 2 and 9 are the homogenized region of carbon and iron used in the previous problem. The zones 3, 5 and 7 are regions of pure iron (atomic density of 9.3692×10^{22}) with 4.25 cm thicknesses, respectively. The zones 4, 6 and 8 are pure carbon (density of 9.3692×10^{22}) with 0.75 cm thicknesses, respectively.

The calculational flow for the problem is shown in Fig. 5.3.2 and the sample input data are given in Tables 5.3.1 to 5.3.4.

Macroscopic cross sections for pure carbon and iron are produced in the step 2 of MACS. In this process, it is assuemd that the number densities for each material are set to unity. Therefore, actual densities for each material are given by density factors (21* array) of ANISN-JR input. In ANISN-JR calculation, volume-flux weighted cross sections are produced for homogenized zones 1, 2 and 9, and for a heterogeneous regions including zones from zone 3 to zone 8.

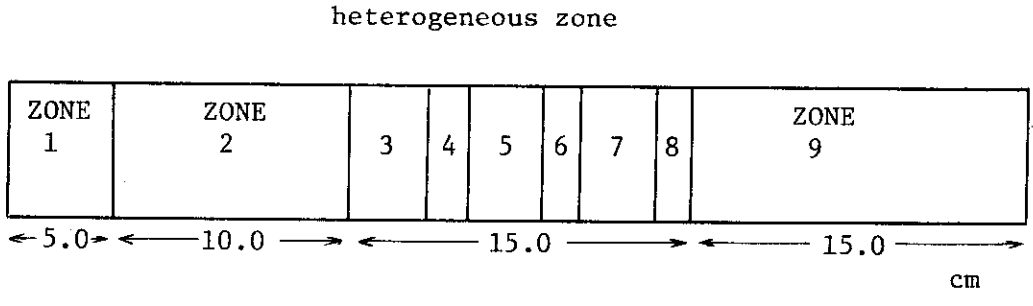

Fig. 5.3.1 On-dimensional calculational geometry of the sample problem No.3. Zones 1, 2 and 9 are the same homogenized mixture as for the sample problem No.2. Zones 3, 5 and 7 are pure iron with atomic density of 9.3692×10^{22}. Zones 4, 6 and 8 are pure carbon with density of 9.3692×10^{22}. The fixed source is distributed in the zone 1 with the density factor of 0.7.

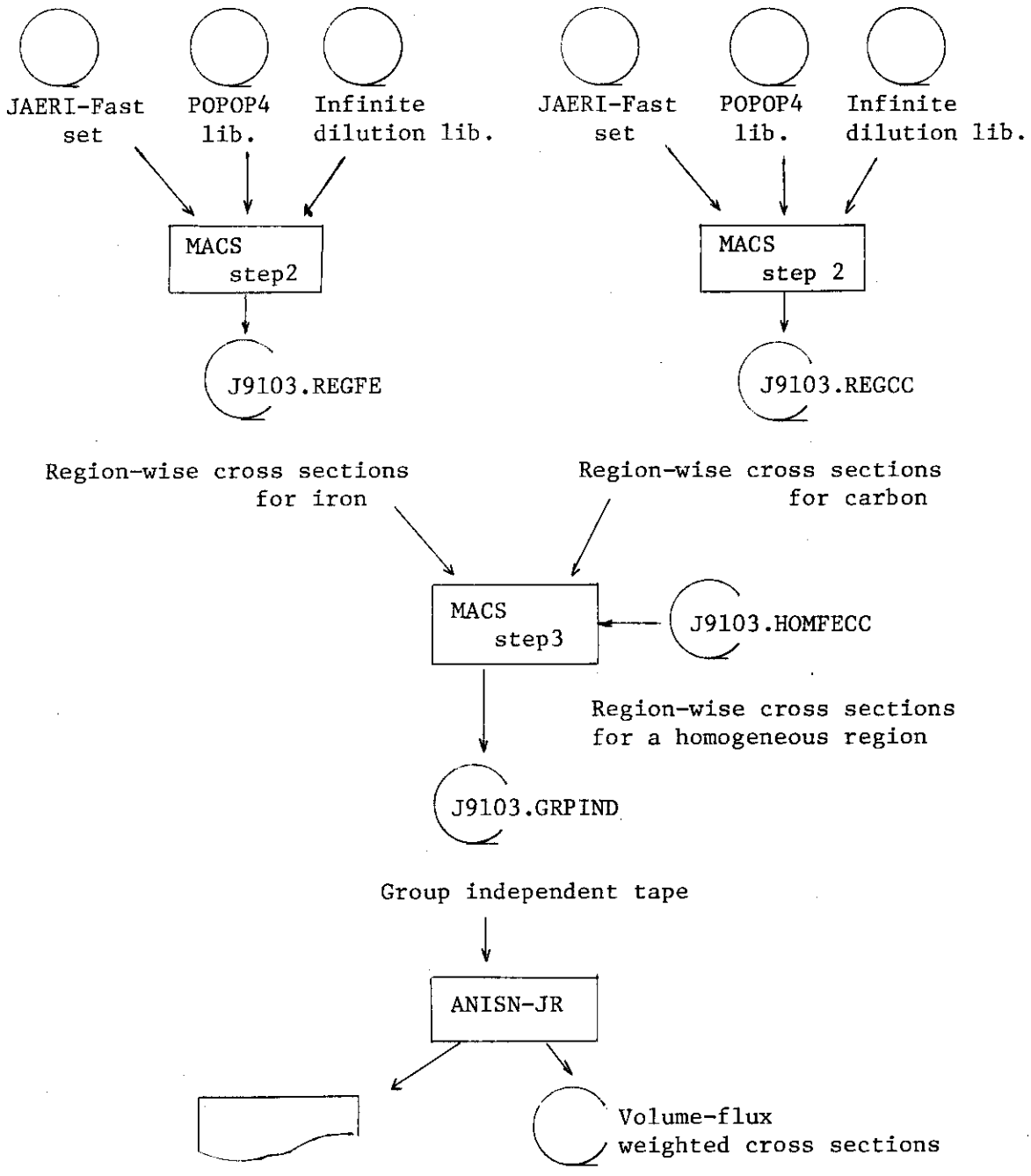

Fig. 5.3.2 Calculational Flow of the sample problem No.3

Table 5.3.1 Input data of the sample problem No.3 to generate macroscopic cross sections for pure carbon by using the step 2 of MACS

```
*HRUN  EFNAME=J9103,RADHEAT3,SIZE=20
*DISK      F01
*DISKTO    F10,J9103,POPBIN2
*DISK      F11
*DISK      F12
*DISK      F13
*DISK      F14
*DISKTN    F15,J9103,REGFE,TRK=20
*DISKTO    F20,J9103,INFLIB
*DISKTO    F41,J9103,JFSET25
*DATA
 1**  2  1  26  8  3  T
 2** 1,5+7 1,05+7 6,5+6 4,0+6 2,5+6 1,4+6 8,0+5 4,0+5 2,0+5 1,0+5
     4,65+4 2,15+4 1,00+4 4,65+3 2,15+3 1,00+3 4,65+2 2,15+2 1,00+2
     4,65+1 2,15+1 1,00+1 4,65  2,15  1,00  4,65-1 1,00-3
 3** 10,2+6 8,0+6 6,0+6 4,0+6 2,5+6 1,2+6 5,0+5 1,0+5 1,0+4
  T
  IRON  CELL
 4**  0  1  1  1  1
 5**  1192
 7**    26
 8**    26,0
 9**  1,00
10**   300,0
  T
12**  25  0  T
13**  1192  2  2  0  1  T
14**  266301  269102  T
17**  1  10  0  1  9  5R0  T
19**  10,2 8,0 6,0 4,0 2,5 1,2 0,5 0,1 0,01
20**  F1,0  T
29**  30  0  0  1  1  T
```

Table 5.3.2 Input data of the sample problem No.3 to generate macroscopic cross sections for pure iron by using the step 2 of MACS

```
*HRUN  EFNAME=J9103,RADHEAT3,SIZE=20
*DISK      F01
*DISKTO    F10,J9103.POPBIN2
*DISK      F11
*DISK      F12
*DISK      F13
*DISK      F14
*DISKTN    F15,J9103.REGCC,TRK=20
*DISKTO    F20,J9103,INFLIB
*DISKTO    F41,J9103,JFSET25
*DATA
 1**  2  1  26  8  3  T
 2** 1,5+7 1,05+7 6,5+6 4,0+6 2,5+6 1,4+6 8,0+5 4,0+5 2,0+5 1,0+5
     4,65+4 2,15+4 1,00+4 4,65+3 2,15+3 1,00+3 4,65+2 2,15+2 1,00+2
     4,65+1 2,15+1 1,00+1 4,65  2,15  1,00  4,65-1 1,00-3
 3** 10,2+6 8,0+6 6,0+6 4,0+6 2,5+6 1,2+6 5,0+5 1,0+5 1,0+4
  T
  CARBON CELL
 4**  0  1  1  1  1
 5**  1274
 7**    6
 8**    6,0
 9**  1,00
10**   300,0
  T
12**  25  0  T
13**  1274  2  2  0  1  T
14**  60102  60304  T
17**  1  10  0  1  9  5R0  T
19**  10,2 8,0 6,0 4,0 2,5 1,2 0,5 0,1 0,01
20**  F1,0  T
29**  20  0  0  1  1  T
```

Table 5.3.3 Input data of the sample problem No.3 to generate a group independent tape for ANISN-JR by using the step 3 of MACS

```
*HRUN  EFNAME=J9103,RADHEAT3,SIZE=20
*DISK      F01
*DISK      F02
*DISKTO    F10,J9103,HOMFECC
*DISKTO    F11,J9103,REGCC
*DISKTO    F12,J9103,REGFE
*DFDISK    F40,J9103,GRPIND,TRK=20,RSIZE=180,BSIZE=3600
*DATA
 1**   3   3   26   8   3   T
  T
30**   0   2   0   T
31**   10   11   12
32**   10   20   30
  T
```

Table 5.3.4 Input data of the sample problem No.3 to produce volume-flux weighted cross sections by using ANISN-JR

```
*HFORT
      COMMON /BULKBU/D(1),LIM1,DUM( 40000)
      LIM1= 40000
      CALL ANISN
      STOP
      END
*HLIED RFNAME=J9103,ANISNJR,EDIT=YES,B=NOMAP
SGMT   ANSMS
SELECT (FTMAIN,CLEAR,CONTRL,ERRO,WOT,SPIE,ITIME,CLOCK,ADDR,ANISN)
SGMT   ANS01,CHN=ANSMS
SELECT (PLSNT,FIDO,TP,ADJNT,S804,S805,S814,WOT8,S966,FFREAD)
SGMT   ANS02,CHN=ANSMS
SELECT (GUTS,S807,S810,S821,S824,S833,DT,CELL,S851)
SGMT   ANS03,CHN=ANSMS
SELECT (FINPR,FINPR1,PUNSH,DTFPUN,FLTFX,NWSUB1,NWSUB2,ERRMSG,ACTPRT,    /
      WOTYT)
SGMT   ANS04,CHN=ANS03
SELECT (BT,SUMARY,FACTOR,NWSUB3,NWSUB4)
SGMT   ANS05,CHN=ANS03
SELECT (FEWG,WATE,CONVT,CRATE)
FIN
*HRUN SIZE=20
*DISK       F01
*DISK       F02
*DISKTO     F04,J9103,GRPIND
*DISKTN     F11,J9103,REGCELL
*DATA
    1     0
    0     2     1    34    26     0     0     0     0     0     0
   36
 1,50E+07  1,05E+07  6,50E+06  4,00E+06  2,50E+06  1,40E+06  8,00E+05  4,00E+05
 2,00E+05  1,00E+05  4,65E+04  2,15E+04  1,00E+04  4,65E+03  2,15E+03  1,00E+03
 4,65E+02  2,15E+02  1,00E+02  4,65E+01  2,15E+01  1,00E+01  4,65      2,15
 1,0       4,65E-01  1,00E-03  1,00E+07  8,00E+06  6,00E+06  4,00E+06  2,50E+06
 1,20E+06  5,00E+05  1,00E+05  1,00E+04
```

Table 5.3.4 (continued)

```
    4
   14   22   30   38
  A HETEROGENIOUS CELL CAL,
15**  200  0  3  4  1  1  0  9 60  0 34  5  6 39  0  0 12 12  1  0  1  0
        0 40  1  1  0  0  1  1  0  1  0  1  1  0
16**  1,05  0,01  1.0-4  1,421  0.0  0,0  0,0  1,0  0,0  0,5  5,0-4
      0,01  0,0   0,0
  T
17**
 5R9,5824-4 55R0,0 5R1,6925-2 55R0,0 5R8,4287-2 55R0,0 5R1,7297-1 55R0,0
 5R2,6260-1 55R0,0 5R2,0558-1 55R0,0 5R1,4845-1 55R0,0 5R6,6319-2 55R0,0
 5R2,6377-2 55R0,0 5R1,0467-2 55R0,0 5R3,4358-3 55R0,0 5R1,0915-3 55R0,0
 5R3,4860-4 55R0,0 5R1,1132-4 55R0,0 5R3,4905-5 55R0,0 5R1,1081-5 55R0,0
 5R3,5287-6 55R0,0 5R1,1050-6 55R0,0 5R3,5064-7 55R0,0 5R1,1161-7 55R0,0
  F0,0  T
 3**  F0,0  T
 1**  F0,0
 4**  410,0 915,0 7115,0 1119,25 7120,0 1124,25 7125,0 1129,25 14130,0
      45,0
 5**  F1,0

 6**   0,0          0,1666667   0,3333333   0,3333333   0,1666667
 7**  -0,9367418  -0,8688903  -0,3500212   0,3500212   0,8688903
 8**  5R1  10R2  8R3  2R4  8R5  2R6  8R7  2R8  15R9
 9**  1  1  9  5  9  5  9  5  1
19**  9R3
21**  5R0,7  10R1.0  30R9,3692-2  15R1.0
27**  3  5  6  39  2
28**  3211  34
29**  100  200  6R300  400
  T
```

5.4 Sample Problem No.4 - Mode Conversion of Cross Section Library by TAPE MAKER

The sample input data for the edit and update options of TAPE MAKER are already shown in the section 5.1. Therefore, in Table 5.4.1, the sample input data are shown to convert a binary mode library (standard mode in RADHEAT-V3) to a BCD mode library. In addition, the input data for the inverse conversion are shown in Table 5.4.2.

The forms of the cross section table in the libraries are described in Appendix F in detail.

Table 5.4.1 Input data of the sample problem No.4 to convert the binary mode library (F01) to the BCD mode library (F10)

```
C
C SAMPLE DATA TO CONVERT A INFINITE DILUTION LIBRARY
C     FROM A BINARY MODE TO A BCD MODE
*HLIEDRUN   RENAME=J9103,TAPEMAKE,GLIED=LIED,GRFD=ON,COMLIB=CALL
*DISKIO     F01,J9103.INFLIB
*NLTAPE     F10,VOL=999999,RSIZE=80,BSIZE=3200
*DATA
  CONVERSION FROM BINARY MODE TO BCD MODE
     1      0     26      0      3      0      0      0      0     10
```

Table 5.4.2 Input data of the sample problem No.4 to convert the BCD mode library (F10) to the binary mode library (F40)

```
C
C SAMPLE DATA TO CONVERT A INFINITE DILUTION LIBRARY
C     FROM A BCD MODE TO A BINARY MODE
*HLIEDRUN   RENAME=J9103,TAPEMAKE,GLIED=LIED,GRFD=ON,COMLIB=CALL
*NLTAPE     F10,VOL=999999,RSIZE=80,BSIZE=3200
*DISKIO     F40,J9103.INFLIB,TRK=20
*DATA
  CONVERSION FROM BCD MODE TO BINARY MODE
     1      0     26      0      3      0      0      0     10      0
```

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5.4 Sample Problem No.4 - Mode Conversion of Cross Section Library by TAPE MAKER

The sample input data for the edit and update options of TAPE MAKER are already shown in the section 5.1. Therefore, in Table 5.4.1, the sample input data are shown to convert a binary mode library (standard mode in RADHEAT-V3) to a BCD mode library. In addition, the input data for the inverse conversion are shown in Table 5.4.2.

The forms of the cross section table in the libraries are described in Appendix F in detail.

Table 5.4.1 Input data of the sample problem No.4 to convert the binary mode library (F01) to the BCD mode library (F10)

```
C
C SAMPLE DATA TO CONVERT A INFINITE DILUTION LIBRARY
C     FROM A BINARY MODE TO A BCD MODE
#HLIEDRUN   RFNAME=J9103,TAPEMAKE,GLIED=LIED,GRFD=ON,COMLIB=CALL
#DISKTO     F01,J9103.INFLIB
#NLTAPE     F10,VOL=999999,RSIZE=80,BSIZE=3200
#DATA
  CONVERSION FROM BINARY MODE TO BCD MODE
     1      0     26      0      3      0      0      0      0     10
```

Table 5.4.2 Input data of the sample problem No.4 to convert the BCD mode library (F10) to the binary mode library (F40)

```
C
C SAMPLE DATA TO CONVERT A INFINITE DILUTION LIBRARY
C     FROM A BCD MODE TO A BINARY MODE
#HLIEDRUN   RFNAME=J9103,TAPEMAKE,GLIED=LIED,GRFD=ON,COMLIB=CALL
#NLTAPE     F10,VOL=999999,RSIZE=80,BSIZE=3200
#DISKTO     F40,J9103.INFLIB,TRK=20
#DATA
  CONVERSION FROM BCD MODE TO BINARY MODE
     1      0     26      0      3      0      0      0     10      0
```

Acknowledgment

The authors wish to thank Dr. T. ASAOKA for helpful suggestions and a critical reading of the manuscript.

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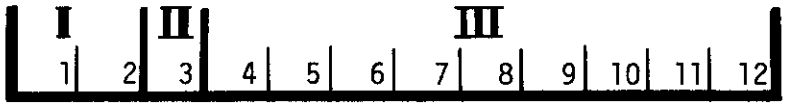
APPENDIX A Free Form FIDO Format(*)

Type 1 Format

Each car is divided up into six 12-digit data fields which are in turn divided up into 3 subfields, as illustrated in the following figure where only one data field is shown.



The first subfield is a two-digit integer; and the second subfield contains either a $, *, R, I, T, S, F, A, C, E, Q, L, N, M, O, U, V, Z, +, -, or a blank. The third subfield contains either a fixed or floating point number. The contents of the first two subfields will define the operation to be performed on the third field.

Blank fields are ignored. One can use any or all fields on a card. For example, a box of blank cards sandwiched anywhere in a data array would be completely ignored.

Each data array is identified by a two-digit integer in a first subfield. There are both fixed and floating point arrays; a fixed point array is designated by a $ in the second subfield, and a floating point array by an *.

The second subfield contains an operator which specifies the type of operation to be performed on the data. The possible operators are listed below.

Array Operators

$ indicates the beginning of an integer array. The first subfield

* All of the descriptions are quoted from Ref. 1).

contains a one- or two-digit number identifying the array.

* indicates the beginning of a floating point array. The first subfield identifies the array.

R indicates that the entry in the third subfield is to be repeated the number of times specified in the first subfield.

I indicates linear interpolation between the entry in the third subfield and the entry in the third subfield of the next data field. The number in the first subfield gives the number of points to be placed equally spaced in the specified range.

T indicates termination of data reading for a block. RADHEAT-V3 can require several data blocks and each block must be ended with a T. A block can contain any number of arrays. Data on a card after a T will be ignored.

S indicates skip. The first subfield defines the number of entries to be skipped. The third field can contain the first entry following the skips. A blank third subfield would be ignored.

F is used to fill the remainder of an array with item given in the third subfield.

A is used to address a particular location in an array. This location is specified in the third subfield, while the first subfield is blank.

C is used to obtain a count of the number of items read into an array up to the point where the C is placed. An integer ZZ in front of the C will be used as identification in producing a message as follows:

XX ENTRIES READ IN THE YY ARRAY at ZZC.

E may be used to end specifying data for an array. This option is particularly useful when it is desired to replace only some items in a particular array. The items in question are replaced, and the use of an E prevents having to count and skip to the end of the array.

Q is used to repeat sequences of numbers. The length of the sequence is defined in the third subfield. The number of times to repeat the sequence is given in the first subfield.

L is similar to I except that a logarithmic interpolation is performed between the entry points. This option is particularly useful for defining energy structures equally spaced in lethargy.

N is used to repeat a sequence of numbers in reverse order. The length of the sequence is defined in the third subfield. The number of times to repeat a sequence is given in the first subfield.

M is used to negate and repeat an inverted sequence. The length of the sequence is given in the third subfield. The number of times to repeat a sequence is given in the first subfield.

O is used to turn on (or off) the card image edit of ANISN input data. As with the C option, an integer in front of the O identifies the particular entry. The default (starting) condition is not to edit the data.

U is used to replace the ANISN input format for an array. The array number is given in the first subfield. The format, written in normal FORTRAN, is specified on the card immediately following the card containing a U. The parentheses normally capsulating a format should be included.

V specifies that the array identified in the first subfield will be read according to the last variable format read in.

Z is used to specify a string of zeroes; e.g., 49Z would place forty-nine zeros into an array.

+ or - indicates exponentiation. The data in the third field is multiplied by $10^{\pm N}$, where N is an integer in the first subfield. This option allows one to specify a number in up to nine significant digits.

Integer data in the third subfield must be right adjusted. Floating point data may be written with or without an exponent. If the decimal is omitted, it is assuemd to be immediately to the left of the exponent field. If there is no exponent, the decimal point is assumed to be to the extreme right of the nine-column subfield.

Input Restrictions

The following restrictions must be observed when using the ANISN input format:

(1) Blank data fields are ignored.

(2) If the interpolation option (I) is used, the next data field may not be either blank or an A entry.

(3) The third subfield of a data field containing a $ or a * may contain an integer N. The next data entry is assumed to be the (N+1)-th member of the array. Normally the third subfield is blank and is ignored.

(4) All data arrays must be filled with the correct number of entries. A data array is ended by either starting a new data array or by ending a data block.

Type 2 Format (Free Form)

The transferral of input data to input forms or punched cards for a code requiring significant amounts of input is always a time consuming, distasteful and error-prone process. The original ANISN formats were designed to help reduce these difficulties. The options are convenience features. The usefulness of the "F" option which fills an array is obvious, but it is somewhat harder to see the practical uses for some of the more obscure ones like N, M, and Q. However, frequent use will turn up situations where these options are invaluable. For example, the S_n cosines are negated and reflected about 90°, a fact of which suggests the use of the M option.

There are justifiable complaints with the input formats; for example, where convenience options are not applicable, data can be hard to write because of the manner in which the data fields are spread on the card. This is especially true of integer arrays, where the data are right adjusted in 12-column fields. The ANISN input forms help to some extent, but the actual key-punching is still troublesome.

This input format has been greatly improved by Ward Engle of ORNL who has designed and implemented an all-FORTRAN free-form ANISN input scheme which has data items separated by blanks (as others do), but still allows all of the important convenience features of the earlier formats. The restrictions on the use of this input are essentially that the user writes the data in a form that he can interpret within the context of the ANISN options. Data is easily written and key-punched, since there is now worry about which type character falls in which column or how many blanks are left between entries.

The free-form input can be interspersed with the fixed form input. To select free-form, an array is identified as either a $$ or a ** array for integer and floating point arrays, respectively.

The restrictions are:

(1) Any third subfield (data entry) must be followed by one or more blanks. This is an obvious restriction, otherwise data interpretation would be impossible.

(2) Only columns 1-72 are used.

(3) Numbers with exponents must not have imbedded blanks; e.g., use 1.0E+4, but not 1.0 E+4 or 1.0E+ 4.

(4) The old + or - options (2nd subfield) are not operational.

(5) No more than 9 digits in a number can be entered. The exponent is not counted; e.g., 9234+09 or 923400000+1 will work, but 9234000000 will not work. Nine-digit accuracy is clearly beyond the significance available for single precision IBM 360 floating point operations.

(6) A blank must not appear between items which fall in the first and second subfields with the old format, e.g., 24R, but not 24 R. Note that the 99 restriction on the number of repeats, interpolations, etc., has been eliminated.

(7) The Z-entry must be entered as 738Z, but not as Z738. The old format allowed either.

(8) The Q, M and N entries must be specified as Q4, but not as 4Q. The old format allows either. An entry like 3Q4 accomplishes the same as Q4 Q4 Q4. This is now true for either format.

The character (') in column 1 of a card will cause the contents of the card to be listed as comments, while the data is read in. Column 2 should contain the proper carriage control character; e.g., blank, 0,1,2, etc. This card is ignored as a data card. This option is also available with the old formats.

Some examples of the new format are given below:

```
1$$25R1_0_4_3Q3_2$$_3R42_E_T
```

The first 25 entries of the 1$ array are 1's followed by 0 and 4, and then the sequence 1 0 4 is repeated three times. The 2$ array has three 42's and then data input to the array ends. The T terminates a data block.

```
42**_0.0_0.1666667_0.3333333_N2
43**_-1.0_-0.8819171_0.3333333 M2
```

This example puts 0.0, 0.1666667, 0.3333333, 0.333333, 0.1666667 in the 42* array and -1.0, -0.8819171, -0.3333333, 0.3333333, 0.8819171 in the 43* array.

Appendix B Descriptions of Subroutines of FFACTOR

B.1 Subroutine FFACTOR

FFACTOR is a control program for calculating the self-shielding factors and effective microscopic cross sections from given atomic densities (9* array) and temperatures (10* array). The infinite dilution cross sections are read from the library tape produced by the STEP1 of the system, and 70-group f-table of the JAERI-Fast set is collapsed into the required energy group structure by using JFUSER.

called from: main routine

subroutin called: XREAD, FREAD, MICRO, XRITE

definition of variables:

NUC : number of materials

MATNO: material identification number given by the STEP1 calculation

MCODE: material identification number given by the JAERI-Fast set (see Appendix D)

IDENT: material identification number given by the THERMOS library

AN : atomic number density

T : temperature (°K)

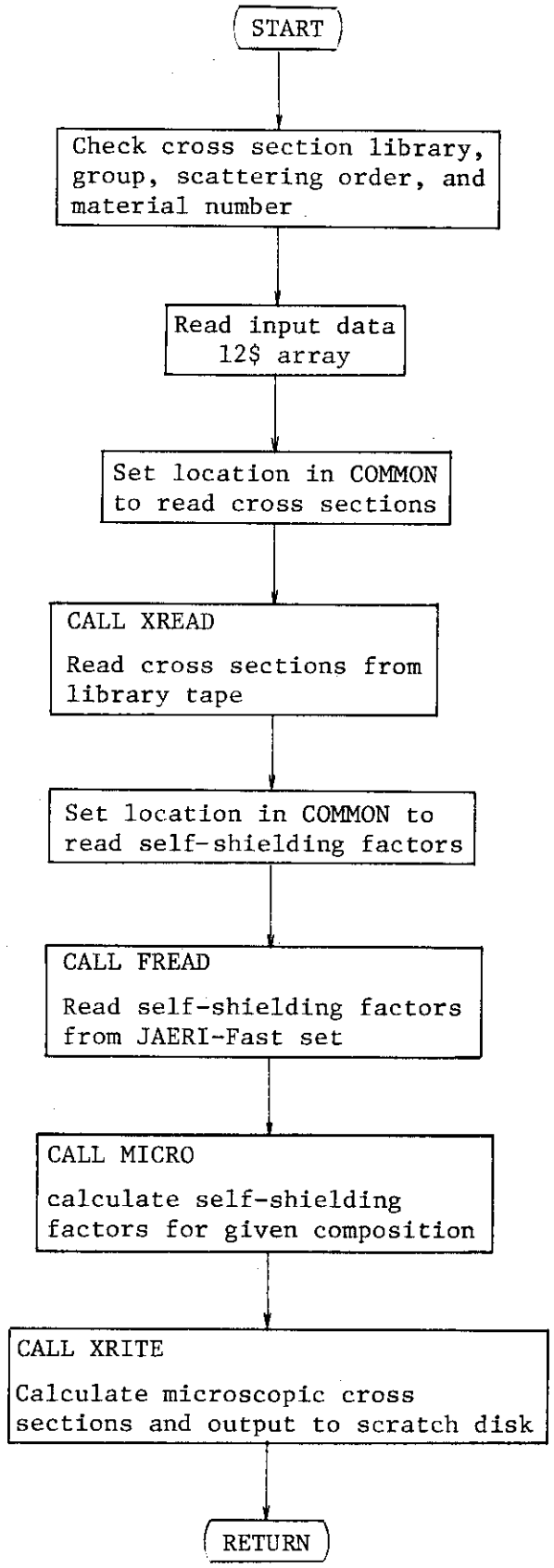
LFCM, LFFM, LFEM and LFRM
: locations of self-shielding factors for capture, fission, elastic and removal reactions

LSSC, LSSF, LSSE, LSSIN and LSS2N
: locations of infinite dilution cross sections for capture, fission, elastic, inelastic and (n,2n) reactions

LSFF1, LSFF2, LSFC1, LSFC2, LSFE1, LSFE2, LSFR1 and LSFR2
: locations of the tables of self-shielding factors for fission, capture, elastic and removal reactions
Number attached at the end of each variable name indicates either R_m table.

NSF : number of materials with the self-shielding factors

Subroutine FFACTOR



B.2 Subroutine MICRO

MICRO interpolates the f-table read by the subroutine FREAD using σ_0^m and temperature of the medium. The σ_0^m is written as follows:

$$\sigma_0^m = \frac{1}{N^m} \sum_{n \neq m} N^n \bar{\sigma}_t^n \qquad (B.1)$$

where N^n is atomic number density of nuclide n, and $\bar{\sigma}_t^n$ the effective total cross section. When material is either ^{235}U, ^{239}Pu, or ^{240}Pu, the contribution of ^{238}U is not added to the sum on the right hand side of Eq. (B.1).

An interpolation for σ_0 is carried out by using a value $X = \log_{10}(\sigma_0+1)$ and a right hyperbolic line as an interpolation function. In this manner, the self-shielding factors, f_c, f_f and f_e, are obtained for capture, fission and elastic scattering reactions, and the effective total cross section $\bar{\sigma}_t$ is calculated from the following equation:

$$\bar{\sigma}_t = f_c\sigma_c + f_f\sigma_f + f_e\sigma_e + \sigma_{in} + \sigma_{n,2n}. \qquad (B.2)$$

After obtained $\bar{\sigma}_t$'s for all nuclides, those values are substituted in Eq. (B.1), and recalculations of $\bar{\sigma}_t$'s are carried out in the same manner. This iteration is executed until the relative deviation of $\bar{\sigma}_t$ becomes less than one percent. When nuclide is either ^{235}U, ^{238}U, ^{239}Pu or ^{240}Pu, also the self-shielding factor for removal reaction is calculated in the same manner.

called from: FFACTOR

subroutine called: SHIELD

definition of variables:

- AN : atomic number density
- T : temperature
- INDEX: location of nuclide on the f-table
- MSF : indication whether nuclide has self-shielding factors or not
- MAXG : number of energy groups
- SSC, SSF, SSE, SSIN and SS2N : cross sections for capture, fission, elastic, inelastic, and (n,2n) reactions
- SFF1, SFF2, SFC1, SFC2, SFE1, SFE2, SFR1 and SFR2 : the table of self-shielding factors for fission, capture, elastic, and removal reactions

FCM, FFM, FEM and FRM

: self-shielding factors for capture, fission, elastic, and removal reactions

TAB1 and TAB2

: σ_0 table converted to the log scale

SST1, SSC1, SSF1 and SSE1

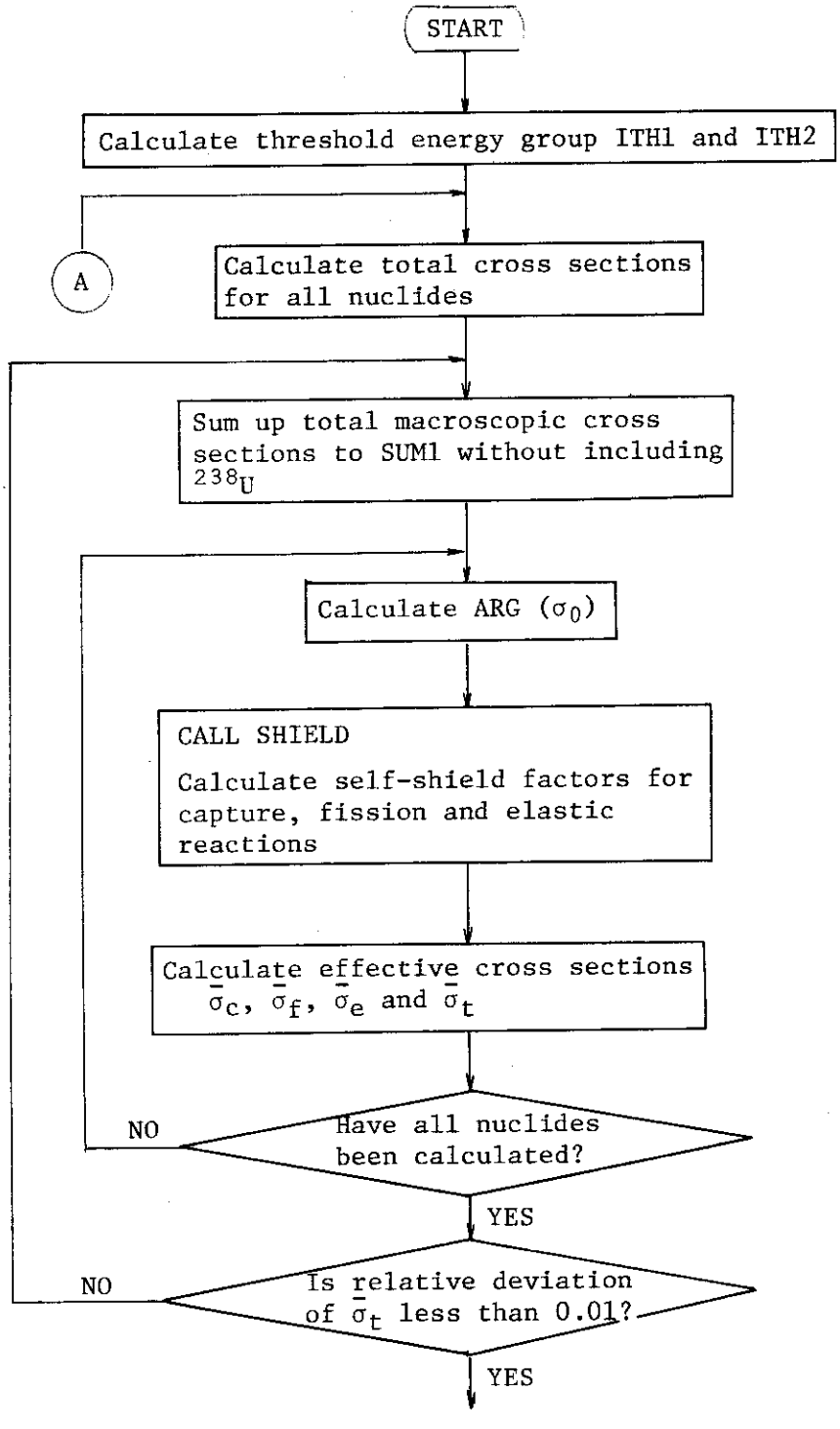
: effective cross sections for total, capture, fission, and elastic reactions

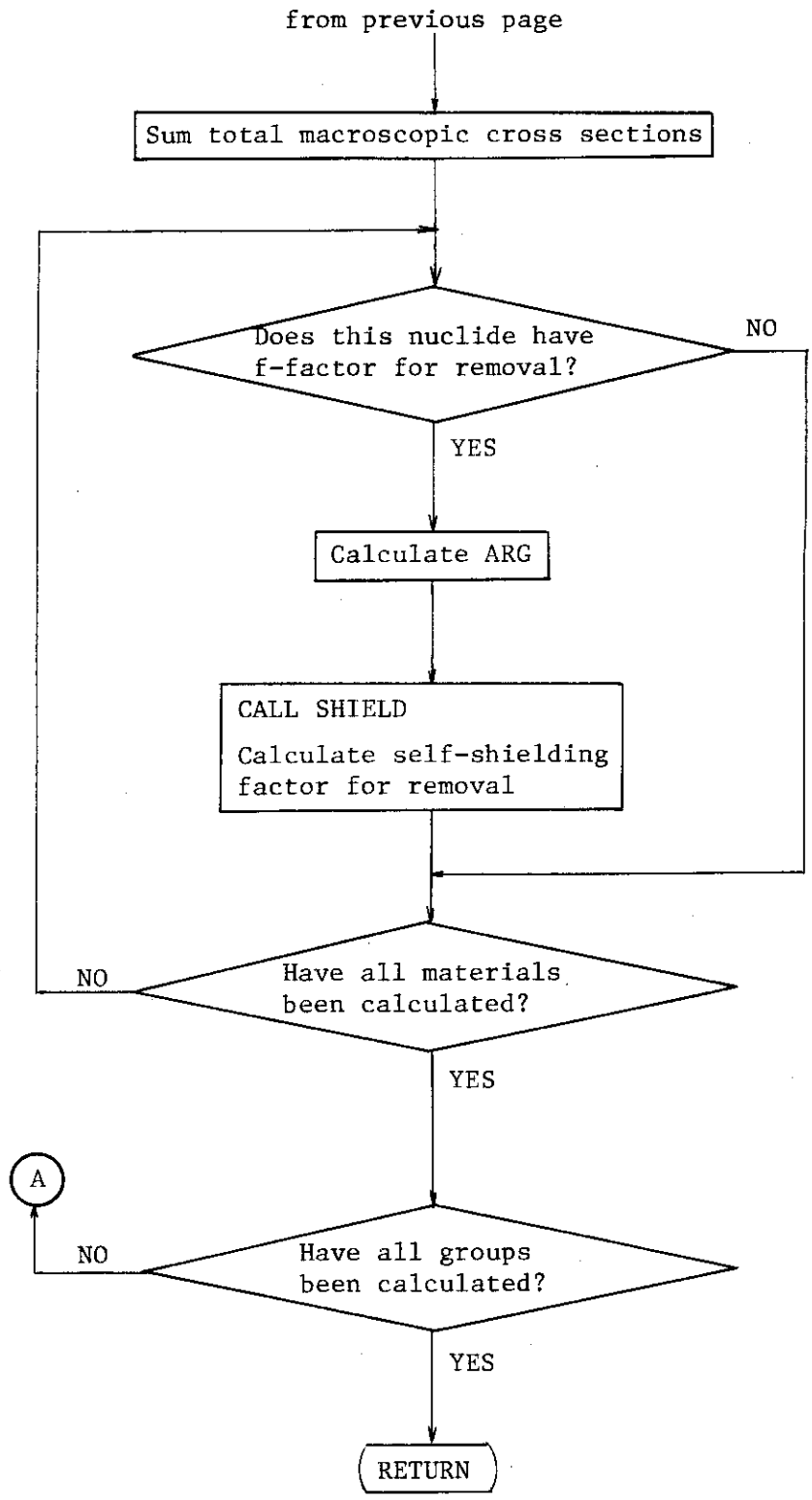
SUM : sum of macroscopic total cross sections for all nuclides

SUM1 : sum of macroscopic total cross sections except ^{238}U

ARG : σ_0

Subroutine MICRO




from previous page
Sum total macroscopic cross sections
Does this nuclide have f-factor for removal?
NO
YES
Calculate ARG
CALL SHIELD
Calculate self-shielding factor for removal
NO
Have all materials been calculated?
YES
A
NO
Have all groups been calculated?
YES
RETURN

B.3 Subroutine XRITE

XRITE calculates effective cross sections, heat generation coefficients, and displacement cross sections by using the self-shielding factors, and writes these values for use in POPOP4 and TOTAL COUPLE. Effective cross sections are calculated from the following equations:

$$\bar{\sigma}_c(g) = f_c(g)\ \sigma_c(g),$$

$$\bar{\sigma}_f(g) = f_f(g)\ \sigma_f(g),$$

$$\bar{\sigma}_e(g) = f_e(g)\ \sigma_e(g),$$

$$\bar{\sigma}_t(g) = \bar{\sigma}_c(g) + \bar{\sigma}_f(g) + \bar{\sigma}_e(g) + \sigma_{in}(g) + \sigma_{n,2n}(g).$$

For nuclides without removal self-shielding factors,

$$\bar{\sigma}_e^{\ell}(g\to g') = f_e(g)\ \sigma_e^{\ell}(g\to g').$$

For nuclides with removal self-shielding factors (^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu),

$$\bar{\sigma}_e^{\ell=0}(g\to g+1) = f_r(g)\ \sigma_e^{\ell=0}(g\to g+1),$$

$$\bar{\sigma}_e^{\ell=0}(g\to g) = \bar{\sigma}_e(g) - \bar{\sigma}_e^{\ell=0}(g\to g+1),$$

$$\sigma_e^{\ell\neq 0}(g\to g') = f_e(g)\ \sigma_e^{\ell\neq 0}(g\to g').$$

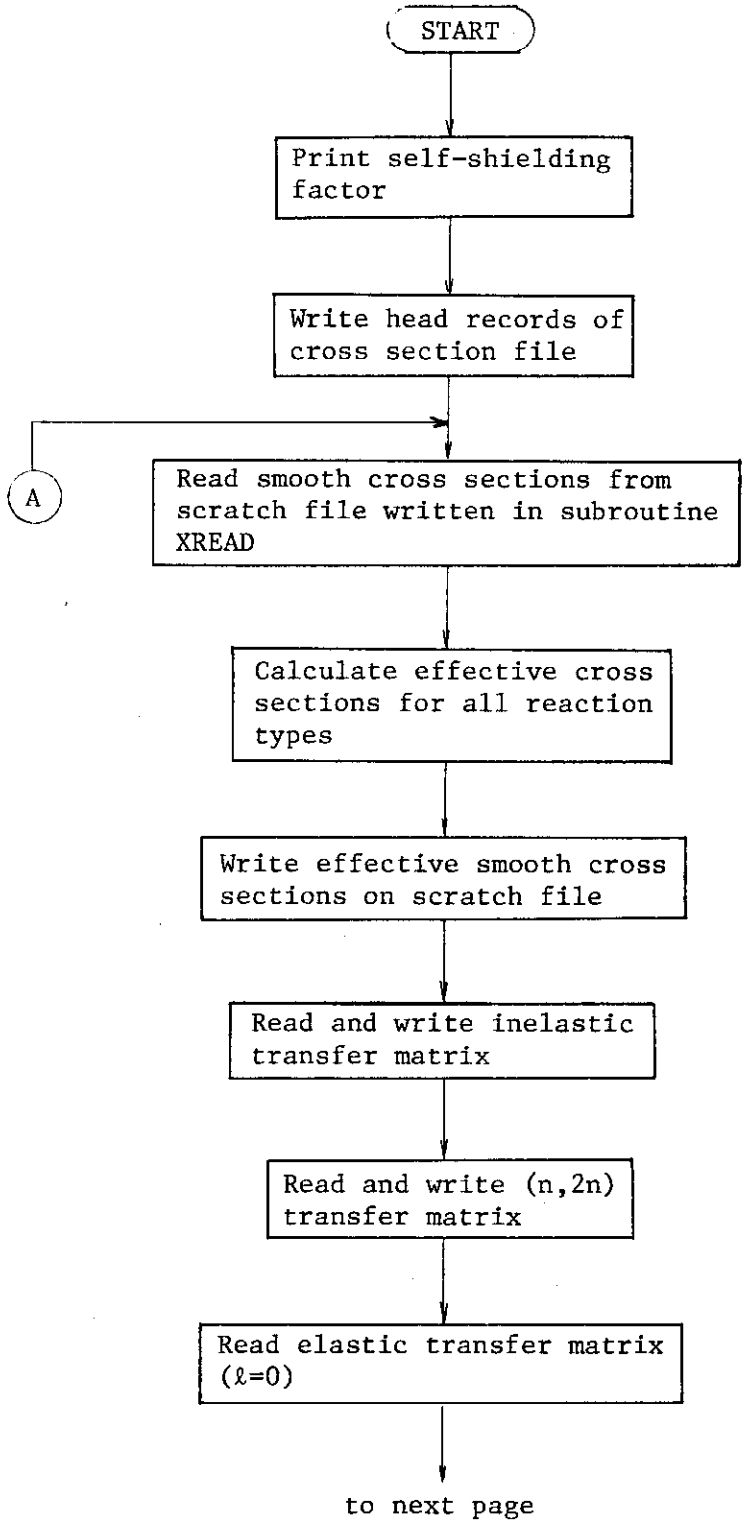
called from: FFACTOR

definition of variables:

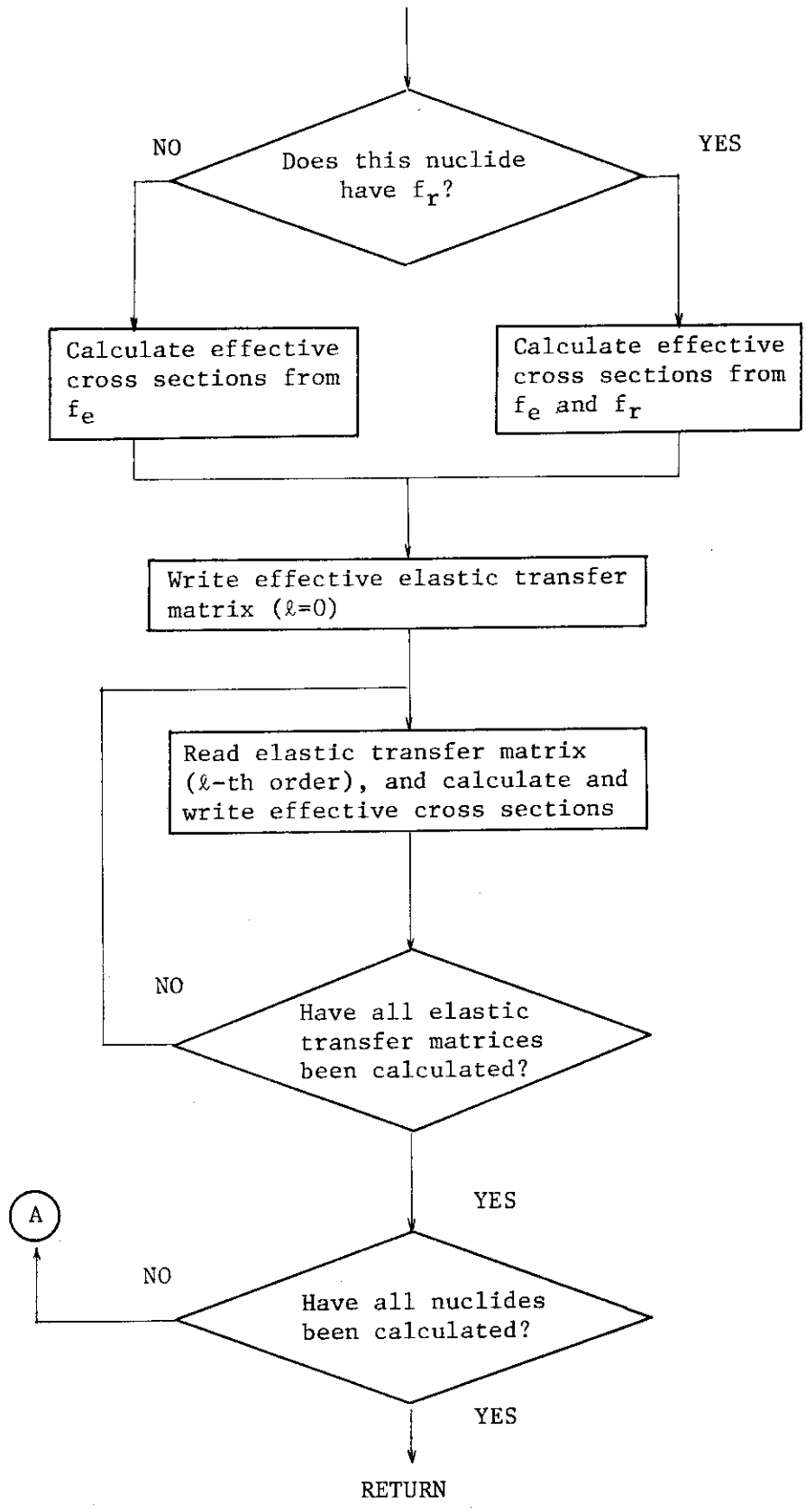
FCM, FFM, FEM and FRM

: self-shielding factors for capture, fission, elastic and removal reactions

Subroutine XRITE



from previous page



B.4 Subroutine XREAD

XREAD reads the infinite dilution library produced in STEP1 (SUPERTOG-JR3). If IOPT = 1 (option for execution of THERMOS) is specified, cross sections of thermal group are replaced by the values calculated in THERMOS. The capture, fission, total elastic, total inelastic and total (n,2n) cross sections used for the calculation of self-shielding factors are stored in the common data area. Cross sections for all nuclides in 5$ array are written on the scratch file for use in the subroutine XRITE.

called from: FFACTOR, MOVEXS

definition of variables:

IMAX: number of energy groups in the infinite dilution library

ITLH: length of cross section table in the infinite dilution library

LOR1: scattering order in the infinite dilution library

MAXG: number of energy groups specified in input data

JTLH: length of cross section table used in this calculation

IPO : scattering order specified in input data

XTHR: thermal cross sections calculated in the THERMOS code, σ_a, σ_f, $\nu\sigma_f$, $\sigma_e^{\ell=0}(g\to g)$ and $\sigma_e^{\ell=1}(g\to g)$

SSC, SSF, SSE, SSIN and SS2N

: cross sections for capture, fission, elastic, inelastic and (n,2n) reactions

B.5 Subroutine FREAD

FREAD reads the f-table from JAERI-Fast set and stores these values to common data area.

called from: FFACTOR

subroutine called: NTABL, SET1 and ADJUST

definition of variables:

INDEX: the location of nuclide on the f-table

ITEMP: indicator whether the required energy group structure is equal to that of the JAERI-Fast set or not

NSF : number of nuclides with self-shielding factors

TAB1 and TAB2

: σ_0 table

SFF1, SFF2, SFC1, SFC2, SFE1, SFE2, SFR1 and SFR2

: the self-shielding tables for fission, capture, elastic and

removal reactions

B.6 Other Subroutines

1) Subroutine MOVEXS

MOVEXS transfers the infinite dilution cross sections from library tape to scratch file. This subroutine is called if IOPT3 (option for execution of FFACTOR) is zero.

called from: main routine

subroutine called: XREAD

2) Function NTABL

NTABL searches the position of the SIGO value on the TAB table.

called from: FREAD

3) Subroutine SHIELD

SHIELD interpolates the f-table by temperature and σ_0. Furthermore, if nuclide is either ^{235}U, ^{239}Pu or ^{240}Pu, the interpolation by R-factor is carry out. When the variable IND is 3, interpolation is performed for f_c, f_f, and f_e-tables, and when IND is 2, interpolation is for f_r-table.

called from: MICRO

subroutine called: ALPHA and BETA

4) Function ALPHA

ALPHA is an interpolating function of a right hyperboilic line. This function is called when three different points are given.

called from: SHIELD

5) Function BETA

BETA is an interpolating function of the same form as in ALPHA. This function is called when only two different points are given.

called from: SHIEDL

6) Subroutine SET1

SET1 sets 1.0 to the self-shielding factor for nuclides without the f-table.

called from: FREAD

7) Subroutine ADJUST

ADJUST interpolates the self-shielding factor according to the input energy structure. The interpolation is carried out for the energy group structure of the JAERI-Fast set.

called from: FREAD

Appendix C Format of JAERI-Fast Set

This library tape is produced for each element in BCD format.

1st record Format (4A4, I4, 12I3, F14.7)

1. Name of element (16 characters)
2. MCODE code number (see Appendix D)
3. MDSE maximum number of the elastic down-scattering groups, where self-scattering is counted as zero-th down-scattering
4. MDSIN maximum number of the inelastic down-scattering groups
   If there is no scattering, MDSIN = 0.
5. MF indicator for a fission material
   0 - no
   1 - yes
6. MSF indicator for f-table
   0 - there is no f-table
   1 - σ_0 = 10^5, 10^4, 10^3, 10^2, 10, 0 (not including σ_0=1)
   2 - σ_0 = 10^4, 10^3, 10^2, 10^1, 1, 0 (including σ_0=1)
7. MTEMP indicator for temperature dependency
   0 - no
   1 - yes
8. MSFMIN first group number where f-table exists
9. MSFMAX last group number where f-table exists
10. MSFF number of f-tables of fission reaction
    0 - none
    1 - only f_1
    2 - f_1 and f_2
11. MSFC same as MSFF except that reaction type is capture
12. MSFE same as MSFF except that reaction type is elastic scattering
13. MSFT same as MSFF except that reaction type is total reaction
14. MSFR same as MSFF except that reaction type is removal
15. AW mass of element

2nd record Format (4E15.5)

$\sigma_t(I)$, $\sigma_f(I)$, $\nu(I)$, $\sigma_c(I)$, I = 1, Maximum number of groups

3rd record Format (4E15.5)

$\sigma_{in}(I)$, $\sigma_e(I)$, $\mu_e(I)$, $\sigma_r(I)$, I = 1, Maximum number of groups

4th Record Format (5E13.5)

There is no record if MDSE = 0

$\sigma_e(I \to 1)$, $\sigma_e(I \to I+1)$, ..., $\sigma_e(I \to I+MDSE)$, I = 1, Maximum number of groups

5th record Format (5E13.5)

There is no record if MDSIN = 0

$\sigma_{in}(I \to I)$, $\sigma_{in}(I \to I+1)$, ..., $\sigma_{in}(I \to I+MDSIN)$, I = 1, Maximum number of group

The following 6th and 7th records are repeated in the order of f_f, f_c, f_e, f_t, and f_r table. If MTEMP = 1, these records are repeated further in the order of 300 °K, 900 °K, and 2100 °K. Furthermore, when the element is either ^{235}U, ^{239}Pu, or ^{240}Pu, these records are repeated twice from samller R. After all, the repetition for the reaction type is innermost and for R is outermost.

6th record Format (E8.1)

Maximum σ_0 of f-table given in next record.

7th record Format (6F8.4)

Self-shielding factors for σ_0 given by 6th record to σ_0 = 0 (maximum 6 values are given). These values are repeated from group MSFMIN to group MSFMAX.

Appendix D JAERI-Fast Set Code Number and Energy Group Structure

D-1 Code number

Order	Element	Code number
1	U-235	925
2	U-238	928
3	Pu-239	939
4	Pu-240	940
5	B-10	105
6	B-11	115
7	C	6
8	O	8
9	Na	11
10	Al	13
11	Cr	14
12	Mn	25
13	Fe	26
14	Ni	28
15	Cu	29
16	Mo	42
17	U-234	924
18	Pu-241	941

D-2 Energy group structure of JAERI-Fast set

ABBN group No.	ΔU	Fine group No.	Δu	Upper energy
1	0.48	1	0.24	10.5 (MeV)
		2	0.24	8.3 (MeV)
2	0.48	3	0.24	6.5 (MeV)
		4	0.24	5.1 (MeV)
3	0.48	5	0.24	4.0 (MeV)
		6	0.24	3.1 (MeV)
4	0.57	7	0.285	2.5 (MeV)
		8	0.285	1.9 (MeV)
5	0.57	9	0.285	1.4 (MeV)
		10	0.285	1.1 (MeV)
6	0.69	11	0.23	0.8 (MeV)
		12	0.23	0.63(MeV)
		13	0.23	0.50(MeV)
7	0.69	14	0.23	0.4 (MeV)
		15	0.23	0.31(MeV)
		16	0.23	0.25(MeV)
8	0.69	17	0.23	0.2 (MeV)
		18	0.23	0.15(MeV)
		19	0.23	0.12(MeV)
9	0.776	20	0.257	100 (KeV)
		21	0.257	77.3 (KeV)
		22	0.252	59.8 (KeV)
10	0.771	23	0.256	46.5 (KeV)
		24	0.258	36.0 (KeV)
		25	0.257	27.8 (KeV)
11	0.761	26	0.254	21.5 (KeV)
		27	0.252	16.6 (KeV)
		28	0.255	12.9 (KeV)
12	0.766	29	0.257	10.0 (KeV)
		30	0.257	7.73(KeV)
		31	0.252	5.98(KeV)
13	0.771	32	0.256	4.65(KeV)
		33	0.258	3.60(KeV)
		34	0.257	2.78(KeV)
14	0.765	35	0.259	2.15(KeV)
		36	0.252	1.66(KeV)
		37	0.255	1.29(KeV)
15	0.766	38	0.257	1000 (eV)
		39	0.257	773 (eV)
		40	0.252	598 (eV)
16	0.771	41	0.256	465 (eV)
		42	0.258	360 (eV)
		43	0.257	278 (eV)
17	0.765	44	0.259	215 (eV)
		45	0.252	166 (eV)
		46	0.255	129 (eV)
18	0.766	47	0.257	100 (eV)
		48	0.257	77.3 (eV)
		49	0.252	59.8 (eV)
19	0.771	50	0.256	46.5 (eV)
		51	0.258	36.0 (eV)
		52	0.257	27.8 (eV)
20	0.765	53	0.259	21.5 (eV)
		54	0.252	16.6 (eV)
		55	0.255	12.9 (eV)
21	0.776	56	0.257	10.0 (eV)
		57	0.257	7.73 (eV)
		58	0.252	5.98 (eV)
22	0.771	59	0.256	4.65 (eV)
		60	0.258	3.60 (eV)
		61	0.257	2.78 (eV)
23	0.765	62	0.259	2.15 (eV)
		63	0.252	1.66 (eV)
		64	0.255	1.29 (eV)
24	0.766	65	0.257	1.0 (eV)
		66	0.257	0.773(eV)
		67	0.252	0.598(eV)
25	0.771	68	0.256	0.465(eV)
		69	0.258	0.360(eV)
		70	0.257	0.278(eV)

Appendix E A Code Number for Reaction Type of POPOP4 Library

The reactions are placed on the library tape in the ascending order of the reaction identification numbers. A possible identifying numbering system would be to use a six-digit integer according to the following scheme:

First and second digits - atomic number of the nucleus

Third digit - the last digit of the target nucleus mass number

Fourth digit - a code for the reaction type e.g.,

0 continuum spectrum

1 (n;γ) nonfission reaction

2 (n;α,γ) reaction

3 (n;n',γ) reaction

4 (n;2n',γ) reaction

5 (n;3n',γ) reaction

6 (n;α,γ) reaction

7 (n;charged particle,γ) reaction

8 (n;γ) fission reaction

Fifth and sixth digits - a code for the source of data. An example of an identification number for the (n;γ) reaction for uranium-238 is therefore 928101. (from Ref. 7))

Appendix F Forms of Cross Section Libraries Produced by RADHEAT-V3

RADHEAT-V3 has three types of cross section libraries. Forms of these libraries are as follows:

F.1 Form No.1: Infinite dilution cross section library

This library is produced by MACS step 1 (SUPERTOG-JR3) and MACS step 2 (FFACTOR), in which the effective microscopic cross sections in a homogenized mixture are generated by taking into consideration of resonance self-shielding effects.

1) The binary mode library is produced as follows:

```
WRITE(20) ING, ING1, LORDER, NUC, (GRP(I), I=1, ING1), (TITLE(I),
   I=1, 12)
WRITE(20) (MATNO(N), N=1, NUC)
DO 20 N=1, NUC
WRITE(20) MATNO(N), (TITLE(I), I=1, 12)
WRITE(20) (σT(I), σc(I), σf(I), ν(I), σnp(I), σnα(I), σnγ(I), σeℓ(I),
   σin(I), σn2n(I), Hf(I), Hnp(I), Hnα(I), Hnγ(I), Heℓ(I), Hin(I),
   Hn2n(I), Dnp(I), Dnα(I), Dnγ(I), Deℓ(I), Din(I), Dn2n(I), I=1, ING)
WRITE(20) (0.0, 0.0, 0.0, (σin(J,I), J=1, ING), I=1, ING)
WRITE(20) (0.0, 0.0, 0.0, (σn2n(J,I), J=1, ING), I=1, ING)
WRITE(20) (σa(I), νσf(I), σT(I), (σeℓ^ℓ=0(J,I), J=1, ING), I=1, ING)
DO 10 L=1, LORDER
WRITE(20) (0.0, 0.0, 0.0, (σeℓ^ℓ=L(J,I), J=1, ING), I=1, ING)
10 CONTINUE
20 CONTINUE
```

where
- ING : number of neutron groups,
- ING1 : ING + 1,
- LORDER: order of Legendre expansion of anisotropic scattering cross sections,
- NUC : number of nuclides in this library,
- GRP(I): neutron energy group structure,
- MATNO : identification numbers of nuclides,
- H(I) : heat generation cross sections,
- D(I) : displacement cross sections,
- σ(J,I): energy transfer cross sections from group J to group I (the form is the same as that of ANISN type cross section beginning with the self-scattering).

2) The BCD mode library is produced as follows:

```
      IO = 20
      WRITE (IO,100)  (TITLE(I), I=1, 12)
      WRITE (IO,200)  ING, LORDER, NUC
      WRITE (IO,300)  GRP(I), I=1, ING1
      WRITE (IO,200)  MATNO(N)=1, NUC)
  100 FORMAT (12A4)
  200 FORMAT (6I12)
  300 FORMAT (1P6E12.4)
      DO 20 N=1, NUC
      WRITE (IO,400)  MATNO(N), (TITLE(I), I=1, 12)
  400 FORMAT (I12, 12A4)
```

This WRITE statement is followed by the same WRITE statements as shown for the binary mode library except for the use of the PUNSH subroutine, in which the output of the cross sections is written in the FIDO form with the R operator (see Appendix A).

F.2 Form No.2: Region-wise cross section library

This type of library is produced by MACS step 2 (TOTAL COUPLE) and by ANISN-JR, in which collapsed cross sections with respect to energy and/or space are generated through the volume-flux weighting for two-dimensional calculations.

1) The elementary form of binary mode library is shown for one material as follows:

```
   1  WRITE(15)  IGM, IHM, IC, MATNO, (TITLE(I), I=1, 12)
      DO 10 I=1, IGM
   2  WRITE(15)  (CRX(J,I), J=1, IHM)
  10  CONTINUE
```

where IGM : number of coupled neutron and gamma-ray energy-groups,
IHM : length of the cross section table CRX,
IC : order of Legendre expansion of anisotropic scattering cross sections.

(Note) Each P_n component is handled as one material in this library, so that the form mentioned above is repeated up to IC+1 times for the complete description of the cross sections expanded into IC components in Legendre polynmials.

2) The elementary form of BCD mode library is shown for one material as follows:

```
      IO = 20
    1 WRITE (IO,100) IGM, IHM, IC, MATNO, (TITLE(I), I=1, 12)
  100 FORMAT (4I6, 12A4)
    2 CALL PUNSH (IO, IGM, IHM, IC, CRX)
```

where the subroutine PUNSH writes the cross sections in the FIDO form with the R operator (see Appendix A).

F.3 Form No.3: Group independent tape

This tape is produced by MACS step 3 as follows:

```
      DO 10 I=1, IGM
      DO 10 M=1, MTP
      WRITE(40) (CRX(J,M,I), J=1, IHM)
   10 CONTINUE
```

where IGM : number of energy groups,

MTP : number of materials in this tape (each P_n component is counted as one material independently),

IHM : length of the cross section table CRX.

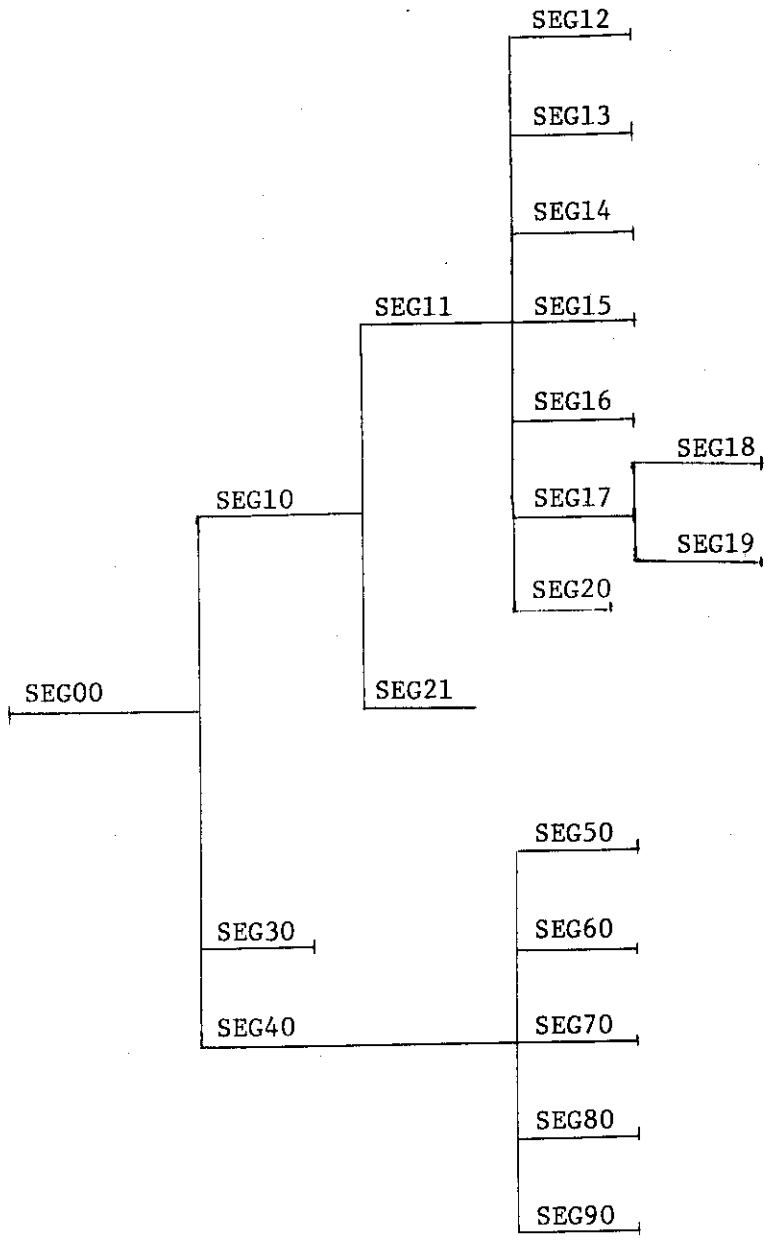
Appendix G Overlay Structure for MACS Code Module and ANISN-JR

G-1 MACS code module

Segment						
SEG00	FTMAIN	PRNAME	FIDOXX	FFREAD	ERRSTP	DFILE
SEG10	SPTOG					
SEG11	ETOG	TPOS	LIST	CONT	TAB1	TAB2
	SAVE	XTND	AVRG	FETCH	STORE	ERROR
	ERR	CRAV	GPAV	ADD	COMB	SUB
	MULT	DIV	TEPR	TERP1	TERP2	LRIDS
	FPDS	IPDS	TERPO	COMBP	GRATE	ECSI
	DELETE	TRID	TMAT	HOLL	TMF3	TMF5
	OUT000	OUT001	OUT002	MISS	GRPAVG	GPAVNW
	XWEIG0	SAVENW	SUBMAX			
SEG12	TMF1	EU	ZERO	ININ	GENT1	OUT1
	KERN	FISS	CHECK	SKPFIL		
SEG13	TMF2	RESS	MASH	VOGAM	TDEGK	
SEG14	RESR	RESU	XSRT	FJ	DLAG	INTER
SEG15	CROS	HSCAT	OUT3	OUT4	OUT6	N2NCRS
SEG16	TRANS	GUTS	GRID	BAST	GADD	TMF4
	RQW8	RQW9	LEGM	INTERP	SUBNW4	PTOFL
	PINTEG	SIMPSN	LEGDD	TABLT2	STELAS	VDIMEN
	FCNTR1	ELAS00	GAUSS	LEGDDN	GNUE	
SEG17	IMAT	RENO	OUT5	SPEC	XSP4	INF5
	CWAX	PUTW	INELAS	LFONE	SUBNW1	SUBNW3
	READIN	EMATRX	SN1N	LEVDEN	AA0AA1	SIGMAC
	HOSEI	CONTUM				
SEG18	FCNTR2	FCNTR3	INELAD	INELA0	GAUSS0	GAUSS1
	TMF5NW	EVAPOF	EVAPOM	GNUE1	GNUE2	GNUE3
	GNUE4	GNUE5	ED4SG	ED4SG1		
SEG19	FCNTR4	NGNPNA	NGFUNC	NPFUNC	NAFUNC	GALT
SEG20	GOUT	PCUT	ADIE	HELGA	IAND	ZAID
	IOR	MASK	ENDFZA			
SEG21	SNOUT	DRAG	ORDER			

G-1 (continued)

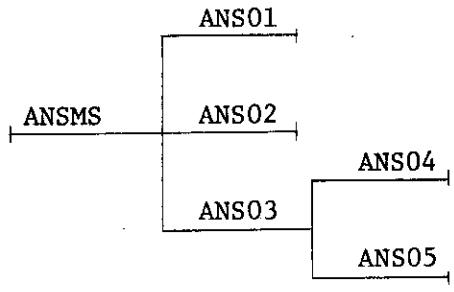
SEG30	THERMS	XSTOP	XPREP	MERGE	GEOMR	GEOMX
	EI	SLABK	ITER	RELAX	EDIT1	EDPREP
	EDIT3	PIJCON	TACKLE			
SEG40	FIDO	WOT	PUNSH	FLTFX	DTFPUN	SIZE
SEG50	FFACTOR	XREAD	FREAD	MICRO	XRITE	SHIELD
	ALPHA	BETA	NTABL	MOVEXS	ADJUST	SET1
SEG60	POPFT	POPOP4	BINEN	FILLY	GAMCOL	GENPRO
	LASTCL	LIBRD	OUTPUT	PHAKE	PHASEI	PHONY
	PLABEL	PUN	SFILLY	SPCASE	TENIPM	TMP4
	TRANSP	WEASEL	YIELD	ERR1	RDMULT	MULT9
SEG70	GAMLEG	GAMS	AL	SIGMAS	SIGLEG	CROSS
	POTO	POTO3	PO6MV1	FUNC1	FUNC2	PAIR
	COHER	NROW	INTFT	INTFK	COMPT	PC
SEG80	TCUP	FRM	RDHD			
SEG90	GRPIN	MRGXS	S805			



SEG10 ∿ SEG21 ——— SUPERTOG-JR
SEG30 ——— THERMOS
SEG50 ——— FFACTOR
SEG60 ——— POPOP4-JR
SEG70 ——— GAMLEG-JR
SEG80 ——— TOTAL COUPLE
SEG90 ——— GROUP-INDEPENDENT

G-2 ANISN-JR

Segment	Subroutine					
ANSMS	FTMAIN ITIME	ANISN CLOCK	CONTRL ADDR	ERRO CLEAR	WOT	SPIE
ANS01	PLSNT S805	FIDO S814	FFREAD WOT8	TP S966	ADJNT	S804
ANS02	GUTS DT	S807 CELL	S810 S851	S821	S824	S833
ANS03	FINPR NWSUB2	FINPR1 ERRMSG	PUNSH ACTPRT	DTFPUN WOTYT	FLTFX	NWSUB1
ANS04	BT	SUMARY	FACTOR	NWSUB3	NWSUB4	
ANS05	FEWG	WATE	CONVT	CRATE		



Appendix H Computer Code Abstract

1. Name of program : RADHEAT-V3
2. Computer for which program is designed : FACOM 230-60/75
3. Nature of physical problem solved : This code system produces the neutron and gamma-ray multigroup cross sections for transport, heat-generation and radiation damage in reactor and shield. Region-wise collapsed few group cross sections are generated from one-dimensional S_n calculations. Treatments are included for resonance self-shielding effect in ABBN type
4. Method of solution : Solution details are discussed in refs. 2 through 14 number item 15 below.
5. Restrictions on the complexity of the problem : The maximum number of neutron groups and gamma-ray groups are respectively 100 and 50. The other restriction is the availability of adequate core storage. All modules excepting SUPERTOG-JR3 are variable dimensioned so that array sizes are set for the particular problem at execution time.
6. Typical machine time : Running times for each job step mainly depend on the following things, (a) step 1 : number of neutron groups and the number of resolved and unresolved resonances. (b) step 2 : number of materials, neutron groups, and gamma-ray groups. (c) step 3 : number of materials, number of coupled energy groups, and order of expansion for the scattering matrices. For step 1, an iron run with 26 neutron groups takes about 1 minutes for generating P_3 cross sections. For step 2 the production of a region-wise iron and carbon coupled neutron-gamma-ray cross sections (26n + 8γ) takes about 10 seconds on the FACOM 230-75 (equivalent to IBM 370/165)
7. Unusual features of the program :
8. Related and auxiliary programs : RADHEAT-V3 produces cross sections compatible with the ANISN-JR, ANISN, DOT, TWOTRAN, and MORSE computer codes.
9. Status :
10. Machine requirement : requires ∿130 Kwords of storage in addition to the usual complement of tapes and direct access devices.
11. Programming language : FACOM 230-75 FORTRAN IV-H. Not include a machine dependent routine.
12. Operating system : FACOM 230-75 MONITOR-VII
13. Other programming information : The program is approximately 24,000

source cards. Overlay structures are employed.

14. User information :

15. Reference :

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3) Honek H.G.: "THERMOS, A Thermalization Transport Theory Code for Reactor Lattice Calculations", BNL-5826 (1961)

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