JAEA-Data/Code
2007-004

JAEA-Data/Code

SRAC2006 : A Comprehensive Neutronics Calculation Code System

Keisuke OKUMURA, Teruhiko KUGO
Kunio KANEKO* and Keichiro TSUCHIHASHI*

Reactor Physics Group
Nuclear Science and Engineering Directorate

February 2007

Japan Atomic Energy Agency

日本原子力研究開発機構

本レポートは日本原子力研究開発機構が不定期に発行する成果報告書です。
本レポートの入手並びに著作権利用に関するお問い合わせは、下記あてにお問い合わせ下さい。
なお、本レポートの全文は日本原子力研究開発機構ホームページ（http://www.jaea.go.jp/index.shtml）より発信されています。このほか財団法人原子力弘済会資料センター*では実費による複写頒布を行っております。

〒319-1195　茨城県那珂郡東海村白方白根2番地4
日本原子力研究開発機構　研究技術情報部　研究技術情報課
電話 029-282-6387, Fax 029-282-5920

*〒319-1195　茨城県那珂郡東海村白方白根2番地4　日本原子力研究開発機構内

This report is issued irregularly by Japan Atomic Energy Agency
Inquiries about availability and/or copyright of this report should be addressed to
Intellectual Resources Section, Intellectual Resources Department,
Japan Atomic Energy Agency
2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195 Japan
Tel +81-29-282-6387, Fax +81-29-282-5920

JAEA-Data/Code 2007-004

SRAC2006 : A Comprehensive Neutronics Calculation Code System

Keisuke OKUMURA, Teruhiko KUGO, Kunio KANEKO[*1] and Keichiro TSUCHIHASHI[*2]

Division of Nuclear Data and Reactor Engineering
Nuclear Science and Engineering Directorate
Japan Atomic Energy Agency
Tokai-mura, Naka-gun, Ibaraki-ken

(Received January 4, 2007)

The SRAC is a code system applicable to neutronics analysis of a variety of reactor types. Since the publication of the second version of the users manual (JAERI-1302) in 1986 for the SRAC system, a number of additions and modifications to the functions and the library data have been made to establish a comprehensive neutronics code system. The current system includes major neutron data libraries (JENDL-3.3, JENDL-3.2, ENDF/B-VII, ENDF/B-VI.8, JEFF-3.1, JEF-2.2, etc.), and integrates five elementary codes for neutron transport and diffusion calculation; PIJ based on the collision probability method applicable to 16 kind of lattice models, S_N transport codes ANISN(1D) and TWOTRAN(2D), diffusion codes TUD(1D) and CITATION(multi-D). The system also includes an auxiliary code COREBN for multi-dimensional core burn-up calculation.

Keywords: SRAC, Neutronics, Reactor Physics, Cell Calculation, Core Calculation, Burn-up Calculation, Resonance Absorption, Group Constants, Collision Probability, S_N, Transport, Diffusion

---

[*1] Integrated Technical Information Research Organization

[*2] retired senior researcher of Japan Atomic Energy Research Institute

SRAC2006：総合核計算コードシステム

日本原子力研究開発機構 原子力基礎工学研究部門
核工学・炉工学ユニット
奥村 啓介、久語 輝彦、金子 邦男[*1]、土橋 敬一郎[*2]

(2007年1月4日受理)

SRAC は様々なタイプの原子炉の炉心解析に適用できる核計算コードシステムである。1986 年に SRAC システムの第 2 版利用手引き（JAERI-1302）が出版された後、多くの機能及びライブラリデータの追加と修正が行われ、総合核計算コードシステムとして完成した。本システムは、主要な核データライブラリ(JENDL-3.3, JENDL-3.2, ENDF/B-VII.0, ENDF/B-VI.8, JEFF-3.1, JEF-2.2 など)と、中性子輸送及び拡散計算のための統合された 5 つの要素コードを含んでいる。それらは、16 種類の格子形状に適用できる衝突確率法に基づく PIJ コード、S_N 法輸送計算コード ANISN（一次元）及び TWOTRAN（二次元）、拡散計算コード TUD（一次元）及び CITATION（多次元）である。また、多次元炉心燃焼計算のための補助コード COREBN がシステムに含まれる。

原子力科学研究所（駐在）：〒319-1195 茨城県那珂郡東海村白方白根 2-4
[*1] 総合技術機構（株）
[*2] 元日本原子力研究所主任研究員

Contents

目　次

1. General Descriptions

1.1 Functions and Features

The SRAC system is designed to permit neutronics calculation for various types of thermal reactors. The system covers production of effective microscopic and macroscopic group cross-sections, and static cell and core calculations including burn-up analyses. The key parameters required in reactor design or experimental analysis are also provided. The present system, however, does not cover problems for photon transport, kinetics and coupling with thermal-hydraulics. The features of the system are in the following;

- Several neutron cross-section libraries based on the latest JENDL, JEFF(JEF) and ENDF/B files are available for more than 300 nuclides.
- The collision probability method code (PIJ) applicable to 16 types of geometries covers cell calculations for most of existing reactors.
- User can compose his own calculational scheme by selecting and combining appropriate codes or optional functions in the system. For example, a variety of the transport codes are available for cell calculations (PIJ, 1D and 2D S_N codes). For core calculations, 1D, 2D and 3D diffusion codes in addition to the above transport codes are also available. Interfacing of cross-section data between the codes is automatically done.
- Three options are available for the resonance absorption calculation in the dominant resonance energy range. The effective cross-sections by the conventional table look-up method based on the narrow resonance (NR) approximation can be replaced by those based on the intermediate resonance (IR) approximation. Moreover a rigorous method is also provided by an optional routine PEACO which solves a multi-region cell problem by the collision probability method using an almost continuous (hyper-fine) energy group structure for the resonance energy range. The interaction of resonances can be accurately treated by the PEACO routine.
- Arbitrary temperature of composite materials is allowed by the interpolation of resonance shielding factors and thermal scattering matrices. For the PEACO routine, Doppler broaden cross-sections in hyper-fine energy structure are internally calculated from the point-wise cross-sections at room temperature.
- The Dancoff correction factor required in the interpolation of the self-shielding factors of

resonance nuclides is automatically calculated by the installed collision probability routines. The factor is given not for an absorber lump but for each constituent nuclide for the cell which contains a resonant nuclide in two or more materials with different compositions.

- A doubly heterogeneous system can be solved by successive cell calculations since homogenizing and collapsing of macroscopic cross-sections is carried out separately. Especially, the resonance absorption of which double heterogeneity effect should be solved simultaneously, can be treated as far as the microscopic cell can be approximated by any of 1D cells.
- The SRAC system can be executed on most of computers with the UNIX operating system or its similar ones like Linux or FreeBSD. Installation of the system is easily done with an equipped installation command which prepares appropriate source programs and other necessary data depending on user's machine.

This report is the fourth edition of the SRAC users manual. A number of additions and modifications to the functions and the library data for the old versions[1)-3)] of SRAC have been made to establish the comprehensive neutronics code system SRAC 2006.

1.2 System Structure

Figure 1.2-1 shows the structure of the SRAC system. The body code of the SRAC integrates the following three transport and two diffusion codes for neutron flux calculations.

- PIJ : Collision probability method code developed at JAERI (current JAEA) which covers 16 lattice geometries shown in Fig.1.2-2,
- ANISN[4)] : One-dimensional S_N transport code which covers slab (X), cylinder (R), and sphere (R_S) geometries,
- TWOTRAN[5)] : Two-dimensional S_N transport code which covers slab (X-Y), cylinder (R-Z), and circle (R-θ) geometries,
- TUD : One-dimensional diffusion code developed at JAERI, which covers slab (X), cylinder (R), and sphere (R_S) geometries,
- CITATION[6)] : Multi-dimensional diffusion code which covers 12 types of geometries including triangular and hexagonal spatial mesh divisions.

For the imported codes ANISN, TWOTAN, and CITATION, several modifications are added for speedup on vector computers, for interfacing of cross-sections between codes, and for our additional functions, while several original functions are suppressed. As far as flux calculation is concerned,

essential programs of the integrated codes are the same as the original ones.

The optional functions to yield effective resonance cross-sections, to calculate depletion of nuclides, reaction rate, etc. are also included. Together with the integrated codes above, various types of fixed source and eigenvalue problems (cf. Sect.1.7) can be solved. The I/O data files for group cross-sections and neutron fluxes are written in the common format called PDS files (cf. Sect.1.4) among the codes. The information written by a code can be read by the succeeding codes.

The function to calculate effective resonance cross-sections (cf. Sect.1.6) includes three options: the NR approximation, the IR approximation, and the hyper-fine energy group calculation by the PEACO[7] routine based on the collision probability method. One of them is chosen by the problem type, required accuracy and computation cost. The function BURN (cf. Sect.1.9) calculates the change of nuclide composition during burn-up by a series of procedures to get a neutron spectrum by a selected code, to get one-group effective cross-sections and to calculate generation and incineration of nuclides at each burn-up step. The reaction rate calculation function REACT (cf. Sect.2.9) provides the spatial distribution of microscopic or macroscopic reaction rate and spectrum indices by using neutron flux obtained by a selected code.

The name of the ‘SRAC system’ usually means not only the body code above-mentioned, but also the whole system including the auxiliary code and data libraries descried below. Hereafter, we call the body code as ‘SRAC code’ to distinguish from the system.

The auxiliary code CORERN is a multi-dimensional core burn-up calculation code which consists of the CITATION using the finite difference method and the function to interpolate macroscopic cross-sections. It uses the tabulated cross-sections provided by the cell burn-up calculation option of the SRAC code. The interpolation of the cross-sections is done on three parameters: an exposure and any two instantaneous parameters. Although the original CITATION code has a burn-up calculation function with microscopic cross-sections, it can not be applied to the thermal reactors with strong heterogeneity in a fuel assembly. Therefore, the table interpolation method of macroscopic cross-sections is adopted. The COREBN has been mainly used for the burn-up and fuel managements of the research reactors in JAEA. As for the COREBN code, details are described in a separate report[8].

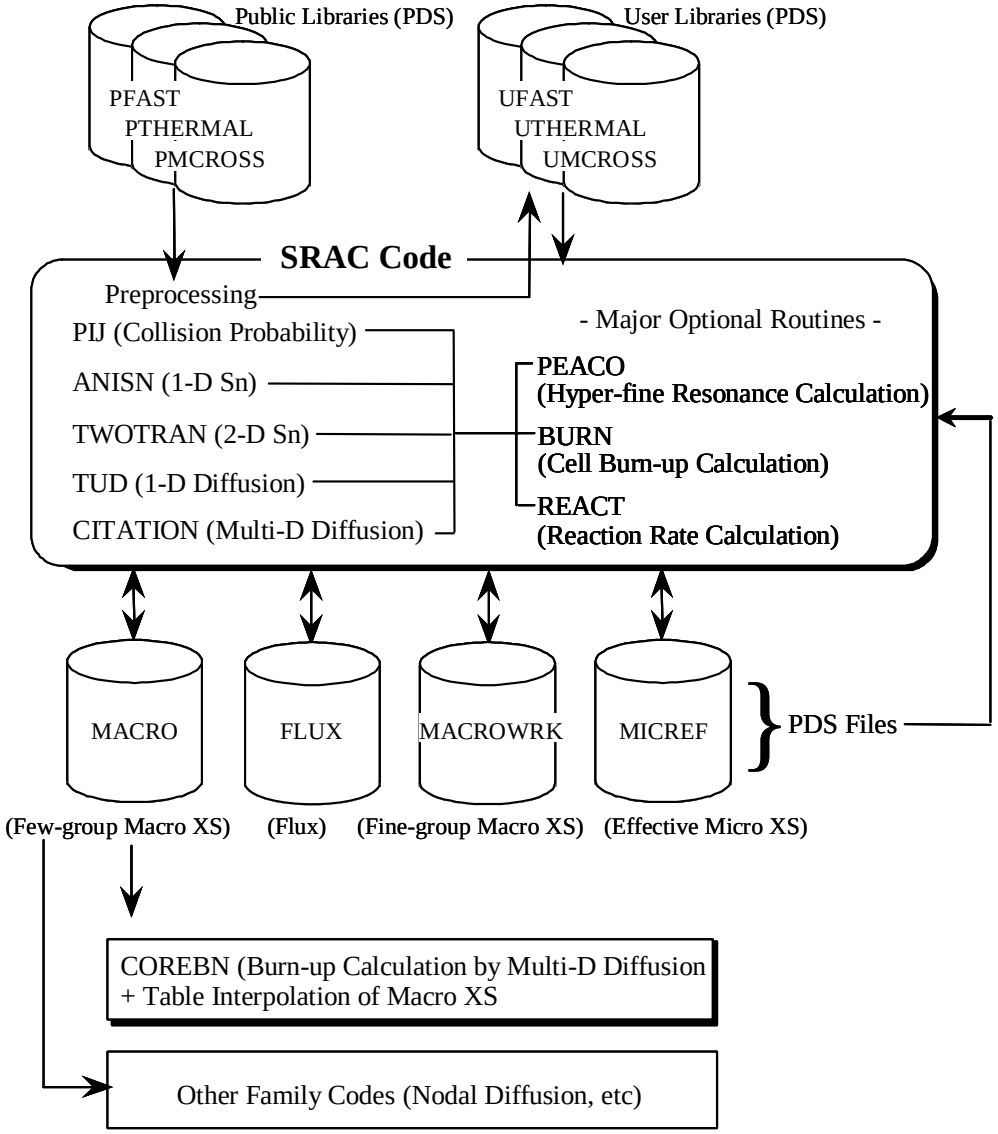
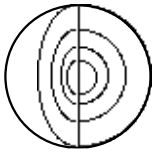
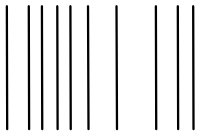


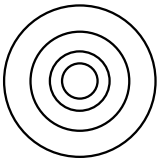
Fig.1.2-1 Structure of the SRAC system



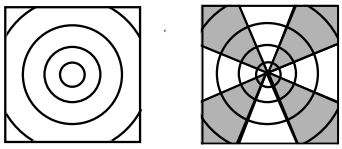
Sphere
(Pebble, HTGR)



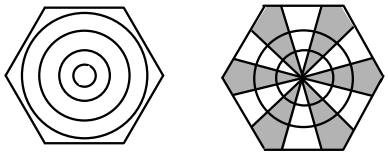
1D-Plate
(JRR, JMTR)



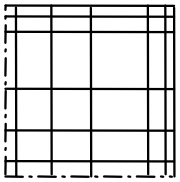
1D-Cylinder
(any pin type fuel)



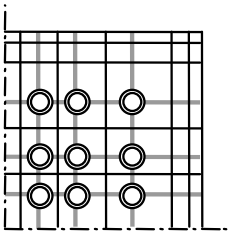
Square unit pin cell
(PWR, BWR)



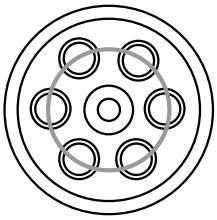
Hexagonal unit pin cell
(FBR, VVER, HCLWR)

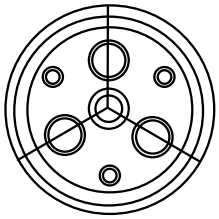


2D square plate fuel assembly (KUCA)

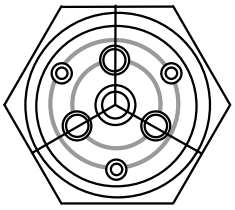


2D square assembly with pin rods (PWR)

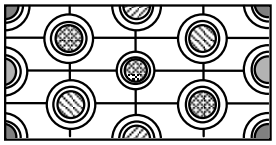




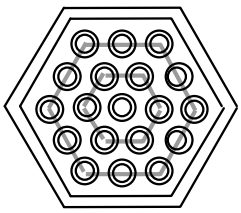
Annular assembly with annular arrays of pin rods
(CANDU, ATR, RBMK)



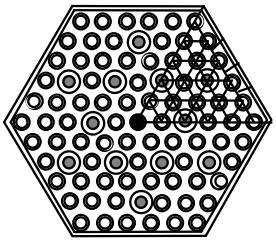
Hexagonal assembly with annular arrays of pin rods (HTTR, VHTRC)



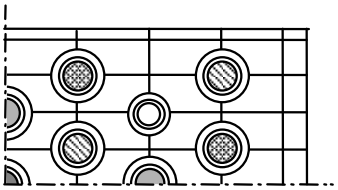
Periodic 2D X-Y array with different pin rods (PROTEUS-LWHCR)



Hexagonal fuel assembly with pin rods (FBR)



Hexagonal Assembly with different types of pin rods (VVER,HCLWR)



Reflective 2D X-Y array with different pin rods (PWR, BWR,etc.)

Fig.1.2-2 Lattice geometry available by collision probability method routine

1.3 Data Libraries

The startup libraries of the SRAC system are organized by three cross-section libraries called as Public Libraries. They consist of Public Fast Library to install fast group cross-sections, Public Thermal Library to install thermal group cross-sections and Public MCROSS Library to install point-wise cross-sections in the resonance energy region which is used by the PEACO routine.

The present system provides several Public Libraries produced from the latest evaluated nuclear data files JENDL-3.3[9], JEFF-3.1[10], ENDF/B-VII[11], etc. by use of nuclear data processing codes LINEAR[12), 13)], RECENT[12), 14)], SIGMA1[12),15)], NJOY99[16)], TIMS-1[17)] and other in-house codes. The user can choose one of the Public Library, or he can make up his own Public library by mixing nuclide-wise data in the Public libraries. The Public Libraries provide the cross-sections which cover the energy range from 1E-5eV to 10MeV for more than 300 nuclides required in neutronics calculation.

Before calculations, the User Libraries (User Fast Library, User Thermal Library and User MCROSS Library) are compiled from the Public Libraries for saving the computer memory and having smooth data access. The User Libraries contain the data of nuclides the user needs in his own energy group structure for his fine-group calculation, where the group constants are automatically collapsed by the asymptotic spectrum (a representative spectrum of thermal reactors) installed in the Public Libraries.

1.3.1 Energy Group Structure and Cut-off-energy

The energy group structure of the current Public libraries consists of 107 groups (74 groups for fast and 48 groups for thermal energy ranges, respectively, with 15 overlapping groups). The energy boundary of each group is shown in Tables 8.3-1 and 8.3-2 in Sect.8.3. The Public Fast Library and the Public Thermal Library cover the cross-section data for neutron energy range 0.41399eV < E < 10MeV and 1E-5eV < E < 3.9279eV, respectively. The user can choose a thermal cut-off-energy from the boundary energies of the fine groups within the overlapping range, that is, 0.41399eV < E < 3.9279eV.

The higher cut-off-energy may be used to take account of the up-scattering of thermal neutron of the material under the high temperature. It should be noted that the cut-off-energy in the SRAC system means the lower energy limit of the PEACO treatment, and the boundary of the switching the cross-section data in the Public Fast and Thermal Libraries. For example, by specifying cut-off-energy below 1eV, the first resonance level of Pu-240 (1.06eV) can be treated by PEACO. This choice of the cut-off-energy is not appropriate for the analysis of light water reactors especially in hot condition,

because the scattering cross-section of the Hydrogen of H_2O in the Public Thermal Library is different from that of the Hydrogen in a free-atom in the Public Fast Library at 1eV. For the continuity of the scattering cross-sections of the compound nuclides (cf. Table 8.1-3), the thermal-cut-off-energy of about 2eV is generally recommended.

1.3.2 Public Fast Library

The fast neutron energy region for the Public Fast Library is defined as the range from 0.41399eV to 10MeV, although the lower energy boundary for the calculation is changeable. The group constants in this energy region are arranged in the form of the cross-section set of the Bondarenko type, that is, the self-shielding factors are given for scattering, removal, capture, fission, and transport cross-sections. The self-shielding factors are tabulated by temperature T and background cross-section σ_0. This form is widely used in fast reactor analysis. The angular dependence of elastic scattering is taken into consideration up to P_5 component depending on nuclide and Library (cf. Sect.8.2). The Public Fast Library has the resonance parameters needed for the IR approximation, and the asymptotic spectrum for collapsing the Public Library into the User Library.

1.3.3 Public MCROSS Library

The effective resonance cross-sections in the energy range of larger than the cut-off-energy can be calculated by the PEACO routine with the collision probability method using an almost continuous energy group structure (at most 19500 energy groups). The upper energy and lethargy mesh are optional: the upper energy is 130.07eV or 961.12eV, the minimum and maximum lethargy mesh (Δu) are 0.00025 and 0.00125, respectively. The Public MCROSS Library has point-wise cross-section data at a room temperature. Before execution of the PEACO routine, the point-wise cross-section is Doppler broadened by the method of SIGMA1[15)] for the temperature of resonant mixture specified by input. After that, the hyper-fine group cross-sections are composed into the User MCROSS Library. The PEACO routine solves a slowing-down equation with it. The MCROSS library data is given for dominant resonant nuclides (cf. Sect.8.2).

1.3.4 Public Thermal Library

The thermal library installs the thermal neutron scattering matrices. The matrices are tabulated on 10 or fewer discrete temperatures ranging from 293K to 2100K. The self-shielding factors are also prepared for the fission and capture cross-sections of the nuclides whose resonance levels exist in the thermal neutron energy region. For some of such nuclides, a representative scattering matrix without temperature dependency is assigned for all the temperatures used in the tabulation of the thermal

library, because of their smaller contributions to neutron energy transfer in practical reactor calculation. In the SRAC calculation, the temperature interpolation is done not only for the resonance shielding factors, but also for the thermal scattering matrices. The interpolation of thermal scattering matrices is made by using the Lagrandian three point interpolation formula[18],

$$\begin{aligned}\sigma(T) = &(T-T_2)(T-T_3)\sigma(T_1)\ /(T_1-T_2)(T_1-T_3)\\ &+(T-T_1)(T-T_3)\sigma(T_2)\ /(T_2-T_1)(T_2-T_3)\\ &+(T-T_1)(T-T_2)\sigma(T_3)\ /(T_3-T_1)(T_3-T_2)\end{aligned} \tag{1.3-1}$$

where, T is the specified material temperature, T_2 is the nearest temperature to T in the tabulated temperature, T_1 and T_2 are the neighboring temperatures of T_2 in the tabulated temperatures. Extrapolation is not available. The scattering matrices are omitted for most of FP (Fission Product) nuclides (cf. Sect.8.2).

1.4 Data Storage in PDS (Partitioned Data Set) Files

In the SRAC system, the integrated codes exchange the information such as cross-sections and fluxes which are stored in the common format file called as PDS file as shown in Fig.1.2-1. PDS file was, originally, the partitioned data set (of only one storied hierarchy) in binary format which is peculiar in the old IBM/FACOM machines with the 'MSP' operating system. Formerly it was an obstacle to export the SRAC system to other machines. As a hierarchical file structure is standard nowadays, the SRAC system is exportable.

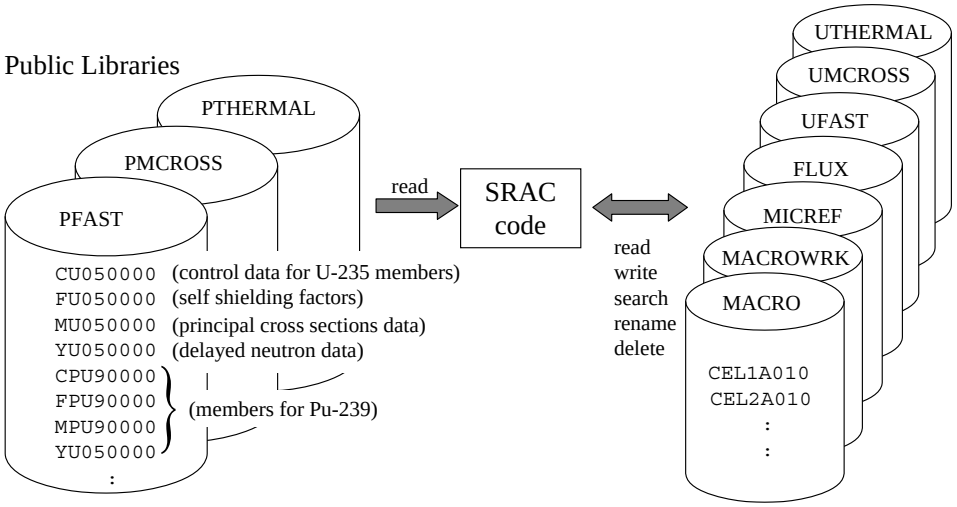


Fig.1.4-1 File I/O with Partitioned Data Set (PDS) files

As shown in Fig.1.4-1, one PDS file can contain a number of sub-files, each of which is called as member. The member name is given by not more than eight alphanumeric characters. In the SRAC system, the role of each constituent character is defined. For example, the Public Fast Library keeps principal cross-section data of U-235 and Pu-239 in the members named as ‘MU050000’ and ‘MPU90000’, respectively. On the UNIX operating system, one PDS file is just a ‘directory’, and a member is a usual sequential access file.

The SRAC code uses the following ten PDS files:

- PFAST : Public Fast Library (read only)
- PMCROSS : Public MCROSS Library for PEACO (read only)
- PTHERMAL : Public Thermal Library (read only)
- UFAST : User Fast Library
- UMCROSS : User MCROSS Library for PEACO
- UTHERMAL : User Thermal Library
- MICREF : Effective microscopic cross sections of mixtures in the fine-group structure of the User Library.
- MACROWRK : Macroscopic cross sections of mixtures and/or those of homogenized materials in the fine-group structure of the User Library.
- MACRO : Macroscopic cross sections of homogenized materials in the few-group structure defined by user.
- FLUX : Flux distribution in the fine-group or few-group structure.

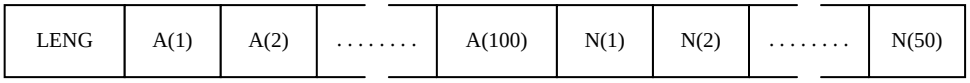
In general, The PDS file has the following advantages:

- A large amount of data can be partitioned by attribution and stored in the member with user-friendly name. In addition, required data can be designated by the member name.
- As the data length of a member is relatively short, it is efficient to read/write data.
- File structure is extendable. It is easy to add new members or PDS files for new concept data.
- File management (deleting, copying, renaming, etc.) is easy. For example, deletion of all members on U-235 in the Public Fast Library can be done by the following UNIX command and masking characters (called meta-character) to specify target member files.

```
rm  ?U05*
```

- Only one logical device is used to access many member files.

Record format of all members is common, although their contents differ. For example, the structure of a member ‘TEST0000’ which has 100 real numbers and 50 integers is as follows.



Here, ‘LENG’ is the total data length in word unit (one word = 4 byte), thus LENG=150 in this case. Data of the member TEST0000 can be read by the following Fortran program.

```
C-------------------------------------------------------------
      DIMENSION A(100),N(50),WORK(200),IWORK(200)
      EQUIVALENCE (WORK(1),IWORK(1))
      OPEN(UNIT=1,FILE='TEST0000',FORM='UNFORMATTED,ACCESS=SEQUENTIAL)
      READ(1) LENG, (WORK(I),I=1,LENG)
      DO I=1,100
        A(I)=WORK(I)
      END DO
      DO I=1,50
        N(I)=IWORK(I+100)
      END DO
      CLOSE(UNIT=1)
C-------------------------------------------------------------
```

Since the SRAC code treats so many members, frequent opening and closing of members causes much execution time. To reduce it, virtual PDS files on the core memory are used during the execution. The members once read by the SRAC code are kept in the virtual PDS files, and after that, the data access to the members is done on the memory. When the total amount of data exceeds the memory capacity secured for the virtual PDS, the data access via virtual PDS is automatically switched to the direct access to the actual PDS. Details on the contents of each member in PDS files and the rule of member name in the SRAC code are described in Sect.3.1.

1.5 Definition of Energy Range

The processing of making the Public Library is dependent on neutron energy range. In the SRAC calculation, the shape of the asymptotic spectrum to collapse the cross-sections of the Public Library into those of the User Library depends on the energy range. Moreover, spatial sub-division for the flux distribution is, in general, changeable by the energy range. Here, the energy range is defined as follows.

1.5.1 Fast Fission Energy Range (10MeV > *E* > 0.82MeV)

This range corresponds to the fast energy region higher than the fission threshold energy of fertile nuclides where the weighting spectrum used for producing the Public Library is assumed to be fission spectrum. The energy averaged spectrum in each group is used as the standard one to collapse the Public Library into the User Library.

1.5.2 Smooth Energy Range (0.82MeV > *E* > 67.4keV)

Since the fluctuations of the various reaction cross-section are rather small in the energy range below about 1MeV, the neutron energy spectrum is smooth, hence the spatial distribution can be assumed to be flat. Though there happen to be some small variations in the neutron spectrum due to the resonance scattering of light and medium weight nuclides, this effect is not so important in thermal reactors. The group constants in the Public Library are processed assuming the neutron spectrum to be $1/\{ E\Sigma(E) \}$, as well as in the following two energy ranges. The $1/E$ spectrum is used as the asymptotic spectrum.

1.5.3 First Resonance Range (67.4keV > *E* > 130eV)

Below about 70keV, fine structure appears in the neutron spectrum due to isolated and/or statistical resonance levels of heavy nuclides, and the Doppler effect must be taken into account. For each heavy resonance nuclide, an exact calculation is made for the resonance shielding factor production using TIMS-1 code[17]. There is, however, no special difference in programming between the smooth and resonance energy ranges in the SRAC system.

1.5.4 Second Resonance Range (130eV > *E* > cut-off-energy)

This energy range corresponds to the lower resonance energy region where are many sharp and strong resonance levels of fissile and fertile nuclides. A special attention must be paid for this range in thermal reactor analyses, because most of resonance absorption occurs in these strong resonances. The resonance shielding factors for a heavy resonant nuclide are evaluated for the homogeneous mixtures with an imaginary nuclide of the constant cross-section. The upper energy boundary of this range is fixed to be 130.07eV, while the lower energy boundary is selected by the user from the group energy boundaries of the Public Library between 3.9279 and 0.41399eV, depending on the problem under study.

The NR approximation is unconditionally used to calculate the effective resonance cross-sections over the all energy ranges. The resonance cross-sections in the second resonance energy range can be optionally replaced by those obtained by the IR approximation or the PEACO calculation.

Formerly the PEACO worked only in the second resonance energy range. Now, the upper energy limit can be extended up to 961.12eV optionally.

1.5.5 Thermal Neutron Energy Range (cut-off-energy > *E* > 1.0E-5eV)

The cut-off-energy should be determined by considering the effect of up-scattering, resonance levels around the cut-off-energy and the continuity of scattering cross-sections described at the previous section. Judging from the comparisons with continuous energy Monte Carlo calculation results, about 2.0eV is recommended, even if sharp resonance levels lower than this energy can not be treated by the PEACO option. The Maxwellian distribution depending on temperature and 1/*E* is assumed for the asymptotic spectrum.

1.6 Effective Resonance Cross-sections

The SRAC code installs three kinds of methods for calculation of effective resonance cross-sections, they are, NR approximation, IR approximation and the PEACO calculation. One of them is selected by the characteristics of the problem, the required accuracy or computation cost. The NR approximation is defaulted unconditionally. If one of other options is specified, the cross-sections obtained by the NR approximation are replaced by the values calculated by the IR or the PEACO calculation, in the energy range where each option is active.

1.6.1 NR Approximation

The Fast and Thermal Libraries contain the infinite dilution cross-sections (σ_∞) of every nuclide and the tabulation of self-shielding factors for resonant nuclides (*f*-table). The effective microscopic cross-section of reaction *x* of nuclide *n* in resonant mixture *i* is given by Eq.(1.6-1) using the above quantities.

$$\sigma^i_{x,n} = \sigma_{\infty,x,n} f_x(\sigma^i_{0,n}, T^i) \tag{1.6-1}$$

where $f_x(\sigma^i_{0,n}, T^i)$ is the resonance self-shielding factor obtained by the interpolation of the *f*-table with a parameter: background cross-section $\sigma^i_{0,n}$ defined by Eq.(1.6-2) and another parameter: the temperature T^i of the mixture of which the nuclide is a constituent. The interpolation is carried out by using the third order spline function. The background cross-section is given by the equivalence theory between homogeneous system and heterogeneous system as

$$\sigma_{0,n}^{i} = \frac{1}{N_n^i} \sum_{m \neq n} (N_m^i \sigma_{t,m}^i) + \frac{g(C_n^i)(1 - C_n^i)}{N_n^i L^i} \tag{1.6-2}$$

$$g(C_n^i) = \frac{a}{1 + (a-1)C_n^i} \tag{1.6-3}$$

where N is the atomic number density, L the mean chord length, C_n the nuclide dependent Dancoff correction factor[19] and a the Bell factor defined in the SRAC code by the geometry of absorbing mixture.

The nuclide dependent Dancoff factor is specified optionally by the input value or the calculated value assuming the black limit in case that the collision probability method is used. The nuclide dependence of Dancoff factor is effective for the lattice including two or more different kinds of resonant mixtures.

The infinite dilution cross-sections are given to the nuclide which has no *f*-table or to every nuclide of the energy group out of range of tabulation. Current available libraries of SRAC have *f*-tables for all resonant nuclides as far as resonance levels are evaluated in nuclear data file. *f*-table is given for the reactions capture, fission, total, elastic, and elastic removal in the fast energy range, and reactions capture, fission and total in the thermal energy range.

Dancoff correction by Tone's method[20] is also available. In this method, the background cross-section is calculated by the following formula;

$$\sigma_{0,n}^{i} = \frac{\sum_j \sum_{m \neq n} N_m^j P_{j \to i} \sigma_{t,m}^j V^j}{\sum_j N_n^j P_{j \to i} V^j}, \tag{1.6-4}$$

where $P_{j \to i}$ collision probability from region j to region i,

V_j volume of region j.

The cell heterogeneity is evaluated so as to consider contributions from each region in a unit fuel cell through collision probabilities. This method is expected to be effective for plate type fuel cell, where a resonant nuclides exists in several composite mixtures with different number densities. It should not be used for a normal pin type fuel cell.

1.6.2 IR Approximation

This method can be applied to the problem where a cell has only one resonant mixture (i=1 only). The microscopic effective resonance cross-sections are given by Eq.(1.6-5) by the interpolation of *f*-table as well as the NR approximation.

$$\sigma_{0,n}^{i} = \frac{1}{N_n^i} \sum_{m \neq n} (\lambda_m N_m^i \sigma_{t,m}^i) + \frac{\mu^* g(C_n^i)(1 - C_n^i)}{N_n^i L^i} \tag{1.6-5}$$

where λ and μ^* are the IR parameters which are obtained by solving the transcendental equations.[21] In the current version, as the energy range where the resonance parameters are prepared for the calculation of the IR parameters is limited from 0.419eV to 130.07eV, the NR approximation is inevitably applied above the upper range even if the IR approximation is selected. The IR approximation is applied to the restricted major fertile nuclides such as Th-232, U-238 and Pu-240.

1.6.3 Direct Calculation on Hyper-fine Energy Group Structure (PEACO)

A direct cell calculation on hyper-fine energy group structure to the heterogeneous lattice cell is available by the collision probability method. The following slowing-down equations on the ultra-fine lethargy mesh (Δu) of about 10^{-3}-10^{-4} are solved by the PEACO routine[7] to obtain the hyper-fine spectra as shown in Fig.1.6-1.

$$V_i \Sigma_i(u) \varphi_i(u) = \sum_{j=1}^{J} P_{ji}(u) V_j \sum_{n=1}^{N} S_{jn}(u) \tag{1.6-6}$$

$$S_{jn}(u) = \frac{1}{1 - \alpha_n} \int_{u - \varepsilon_n}^{u} \exp\{-(u - u')\} \Sigma_{sjn}(u') \varphi_j(u') du' \tag{1.6-7}$$

$$\alpha_n = \left\{ \frac{A_n - 1}{A_n + 1} \right\}^2, \qquad \varepsilon_n = -\ln \alpha_n \tag{1.6-8}$$

where the subscripts *i*, *j* denote the region numbers, *n* the nuclide, $P_{ji}(u)$ the probability that a neutron scattered isotropically in the region *j* has the first collision in region *i*, $S_{jn}(u)$ the slowing-down source. The neutron spectrum $\varphi_i(u)$ is numerically calculated by the recurrence method developed by Kier.[22]

The effective fine-group cross-sections are directly calculated with $\varphi_i(u)$ and hyper-fine cross-sections. The use of the PEACO routine is, in principle, limited to the system which includes one or two different resonance

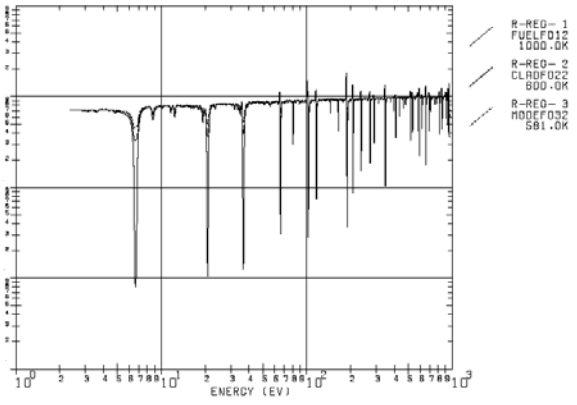


Fig.1.6-1 Neutron spectra by PEACO

mixture(s) having resonant nuclides appearing in the MCROSS Library. It can be, however, extended to the system which includes more than two resonant mixtures as far as several mixtures can be assumed to be the same kind. For the nuclides not compiled in the MCROSS Library, their cross-sections are not corrected by the PEACO routine.

1.7 Fixed Source Mode and Eigenvalue Mode

Each of the integrated code PIJ, ANISN, TWOTRAN, TUD and CITATION works on the following two alternative problem modes.

1.7.1 Fixed Source Mode

The first mode is the fixed source problem mode where a flux calculation is carried out by separating fast groups and thermal groups. The Public (and User) Fast Library installs a fission neutron spectrum as a defaulted source assuming thermal fission of U-235. In the fixed source mode, the fixed source having this spectrum is uniformly distributed in the fuel region, then the spatial and energy distribution of flux in fast groups is solved. After finishing the calculation of fast groups, the slowing-down source into the thermal energy range is calculated, then the thermal flux is iteratively solved. In this mode as described in Sect.1.8, the spatial division may be different between the fast and the thermal ranges if the PIJ code is used. While the spectrum is separately solved in this mode, an optional routine HOMOSP is prepared to calculate the spectrum over the whole energy by using the homogenized cross-sections obtained in the above steps with considering the effect of leakage. In this process the P_1 or B_1 approximation is used to solve the one-point eigenvalue problem with the buckling specified in the input. While the spectrum is modified by considering the leakage, the spatial distribution is preserved as obtained in the fixed source mode calculation. The HOMOSP routine yields the infinite multiplication factor and the effective one corresponding to the buckling, as well as the homogenized spectrum.

1.7.2 Eigenvalue Mode

The second mode is the eigenvalue problem mode where a flux calculation is carried out over the whole energy range. In this mode, the spatial division (R-Region, cf. Sect.1.8) is common over the whole energy groups and fluxes and fission neutron sources are iteratively solved. Therefore, the fission source distribution in this mode is more accurate than that in the first mode. Note that not only the conventional eigenvalue problems but also the external source problems over the whole energy

range are treated in this mode in the flow diagram of the SRAC code.

As the PEACO routine solves the slowing-down equation by the collision probability method only in the resonance energy range, it is not available in the eigenvalue mode or in the fixed source mode by codes except PIJ. In order to use the effective cross-sections obtained by PEACO in the eigenvalue mode, the cross-sections have to be prepared in advance by PIJ with PEACO in the fixed source mode.

1.8 Definition of Spatial Division

In the SRAC code, several spatial divisions called as Sub-Region, T-Region, R-Region, X-Region and M-Region are used. Particularly for cell calculations, various space regions and meshes are defined to enhance the calculation accuracy or to save the computer time, as the needs of the case demand. They are defined as follows;

1.8.1 Sub-Region

The concept of Sub-Region is used only for the PIJ code. The Sub-Region is the purely geometrical sub-division that is bounded by the lines or circles used to identify the location of sub-division under consideration for the collision probability method. The rule of numbering of S-Regions is fixed by geometry model. S-Region is defined for convenience and does not have direct relation with the accuracy of flux calculation.

1.8.2 T-Region

In the fixed source mode, the fast energy range and the thermal energy range are separately solved. Thermal neutron fluxes have steeper gradient than fast neutron fluxes. Therefore, the flux calculation in the thermal energy range requires finer spatial mesh division than in the fast energy range. A unit of spatial division used in thermal flux calculation is called as a T-Region. A T-Region is composed by one or more S-Region(s) taking into account of geometrical symmetry. Some adjacent S-Regions with thin optical thickness can make a T-Region. In the S_N or diffusion codes, the finest spatial mesh is treated as a T-Region.

1.8.3 R-Region

Since the neutron distribution in the fission or resonance energy range is rather flat than in the thermal range, it is not always necessary to sub-divide the geometry into so many meshes as in the

thermal energy range. In the fixed source mode, a unit of spatial division used in fast and resonance flux calculation is called as an R-Region. The user forms an R-Region by collecting several T-Regions estimating the flatness of flux distribution. When the eigenvalue mode is chosen, R-Region is the spatial division in the whole energy range. A material is allocated to each R-Region.

1.8.4 X-Region

A core calculation requires homogenized cross-sections in a lattice cell. Therefore, one or more cell calculations on heterogeneous cell(s) are necessary beforehand the core calculation. Usually the homogenized cross-sections are obtained by the flux-volume weight of cross-sections of constituent materials. An X-region is the range of spatial integration. It is formed by gathering some of the R-regions. The homogenized cross-sections and fluxes used are stored in PDS files.

For usual cases, one X-Region corresponds to whole unit cell of which homogenized cross-sections are provided to the core calculation. An example to use plural X-Regions is the case to calculate the cross-sections of a control rod. As output of a heterogeneous cell calculation of the system including fuel and control rod, one can obtain the cross-sections of the control rod region and those of the neighboring fuel region by allocating these two regions to two separate X-Regions. Another kind of specification is that some of the R-Regions may be excluded from any of the X-regions when they are added as extra regions to an isolated cell to simulate the surrounding boundary condition by allocating zero value to these R-Regions.

1.8.5 M-Region

M-Region is used for allocation of materials. An M-Region is formed by one or more R-Regions which have the same composition. On the calculation of the background cross-section σ_0 based on the NR or IR approximation, the collision probabilities are calculated to the M-Region. Effective microscopic cross-sections are transferred to the burn-up routine by M-Region.

1.9 Cell Burn-up Calculation

In the cell burn-up calculation, burn-up changes of atomic number densities of nuclides in the burn-up chain model is obtained by solving the depletion equation with the reaction rates for fission, capture and (n,2n) reactions. Details on data and method are written in Sect.3.3 and Sect.7.7. SRAC provides several burn-up chain modes, and user can choose the most appropriate model by considering reactor type and his purpose.

The following optional treatments are available in the cell burn-up calculation:

- Option to consider cooling time during burn-up (e.g. analysis of post irradiation examination)
- Option to calculate instantaneous or integrated conversion ratio by user definition
- Burn-up calculation with constant flux level (e.g. burn-up of blanket fuel)
- Branch-off calculation (e.g. Doppler or void reactivity in each burn-up step)
- Burn-up calculation to start by reading the initial composition from a burn-up calculation result in different condition.
- Burn-up calculation with fixed number densities for specified nuclides (e.g. zero Xe in branch-off calculation, or on-line decontamination)
- Restart option to recover a burn-up calculation terminated for any reasons. It is available as far as the MACRO file is preserved.

As well as the atomic number densities along burn-up, the following items are edited for each M-Region and X-Region on the text file allocated to the 98-th logical device.

DAYS	Accumulated burn-up period in days
MWD/T	Exposure (MWt*days per metric-ton of initial heavy metal inventory)
U05-%	Fraction of depleted U-235 (changeable by user) atomic number density to the fresh one (0-100%)
K-EFF	Effective neutron multiplication factor
K-INF	Infinite neutron multiplication factor
INST. C.R.	Instantaneous conversion ratio defined by user
INTE. C.R.	Integrated conversion ratio defined by user
MWD	Exposure (MWt*days)
POWER (MW)	Thermal power over the cell
TON-HM	Heavy metal inventory in metric-ton ($=10^3$kg)
FLUX LEVEL	Absolute one-group flux level (n/cm^2-sec)
FIS. ABSOR.	Macroscopic absorption rate of fissile nuclides defined by user (sec^{-1})
FIS. DECAY	Decay rate of fissile nuclides defined by user (sec^{-1})
FER. CAPT.	Macroscopic capture rate of fertile nuclides defined by user (sec^{-1})
POW (MW/CC)	Power density (MW/cm^3)
ENERGY/FIS.	Average energy release per fission (Joule/fission) weighted by nuclide-wise fission rate
XE-135 YD.	Average fission yield of X-135 weighted by nuclide-wise fission rate
I-135 YD.	Average fission yield of I-135 weighted by nuclide-wise fission rate
SM-149 YD.	Average fission yield of Sm-149 weighted by nuclide-wise fission rate
PM-149 YD.	Average fission yield of Pm-149 weighted by nuclide-wise fission rate

The above data are stored in MACRO file together with few-group macroscopic cross-sections to be used in the COREBN code[8].

1.10 Calculation Scheme

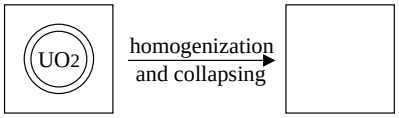
In Fig.1.10-1, a flow diagram of the SRAC code is shown. The number in the brackets '[ ]' in this figure denotes the step number printed on the standard output. The diamond-shaped mark denotes a branching point of the calculation by user options. In this flow, a set of flux calculation named by 4 characters (case name) is repeated until a blank case name is entered. The user can compose his own calculation scheme by combining several cases required for his purpose. The cases can be repeated as far as the computation cost allows. Here, we shall follow the following assuming a typical example.

---------- Specification of the example ----------

First case : UO2F

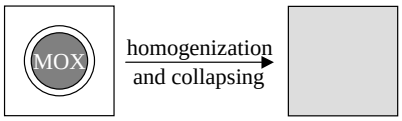
Cell calculation for a pin rod lattice of UO_2 fuel,

- with the JENDL-3.3 library,
- in fine-energy-group structure (e.g. 90 groups),
- in fixed source mode,
- by PIJ with PEACO



Second case : MOXF

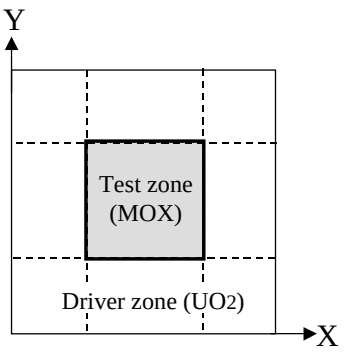
Cell calculation for a pin rod lattice of MOX fuel by the method same as the previous case.



Third case : CORE

Core calculation for a critical assembly where a central test zone of the MOX fuel is surrounded by a driver zone of the UO_2 fuel.

- with the homogenized cross-sections provided by the first and second cases,
- in few-energy-group structure (e.g. 4 groups),
- in eigenvalue mode,
- by CITATION with two-dimensional X-Y model.



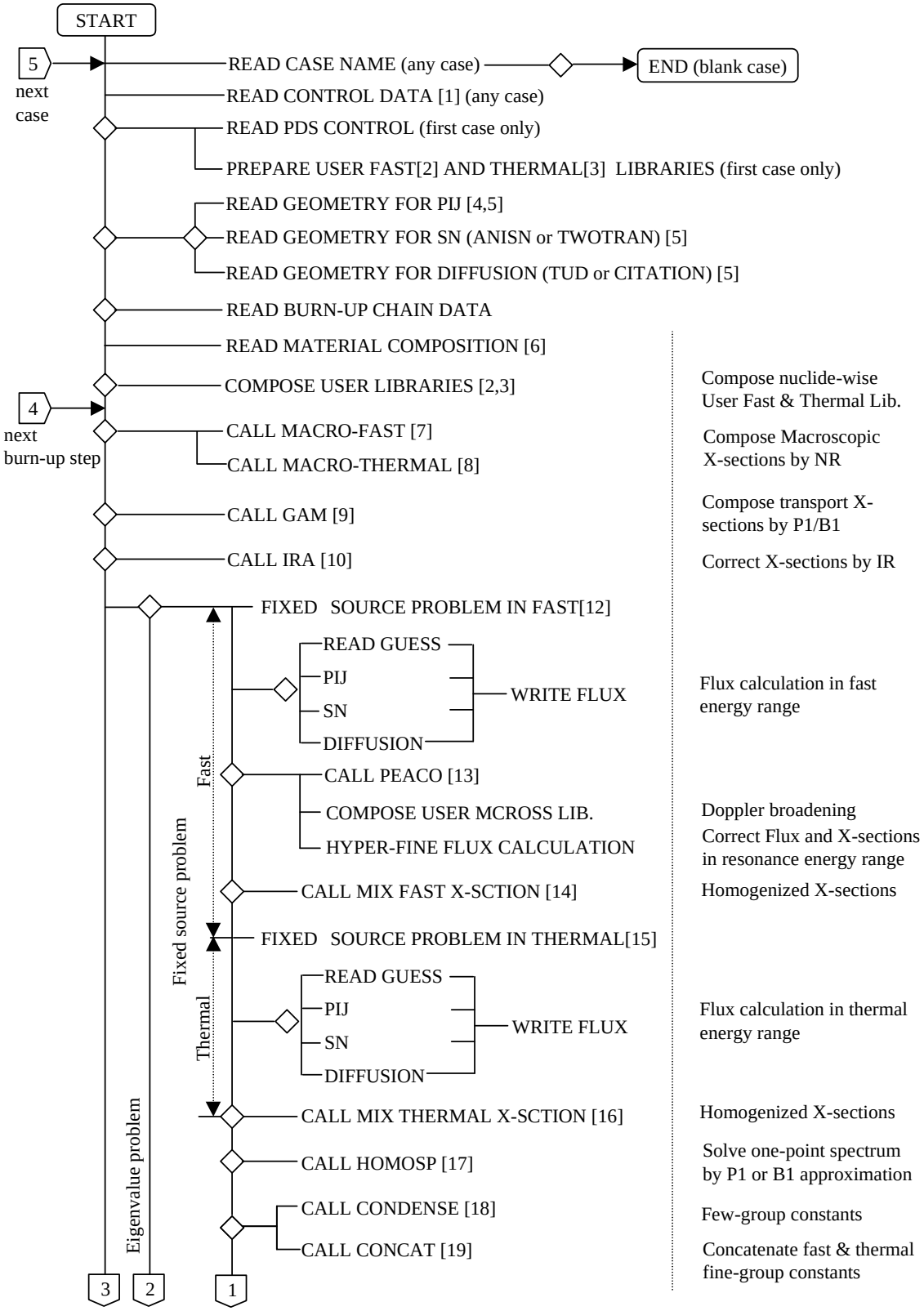


Fig.1.10-1 (1/2) Flow daigram of the SRAC code

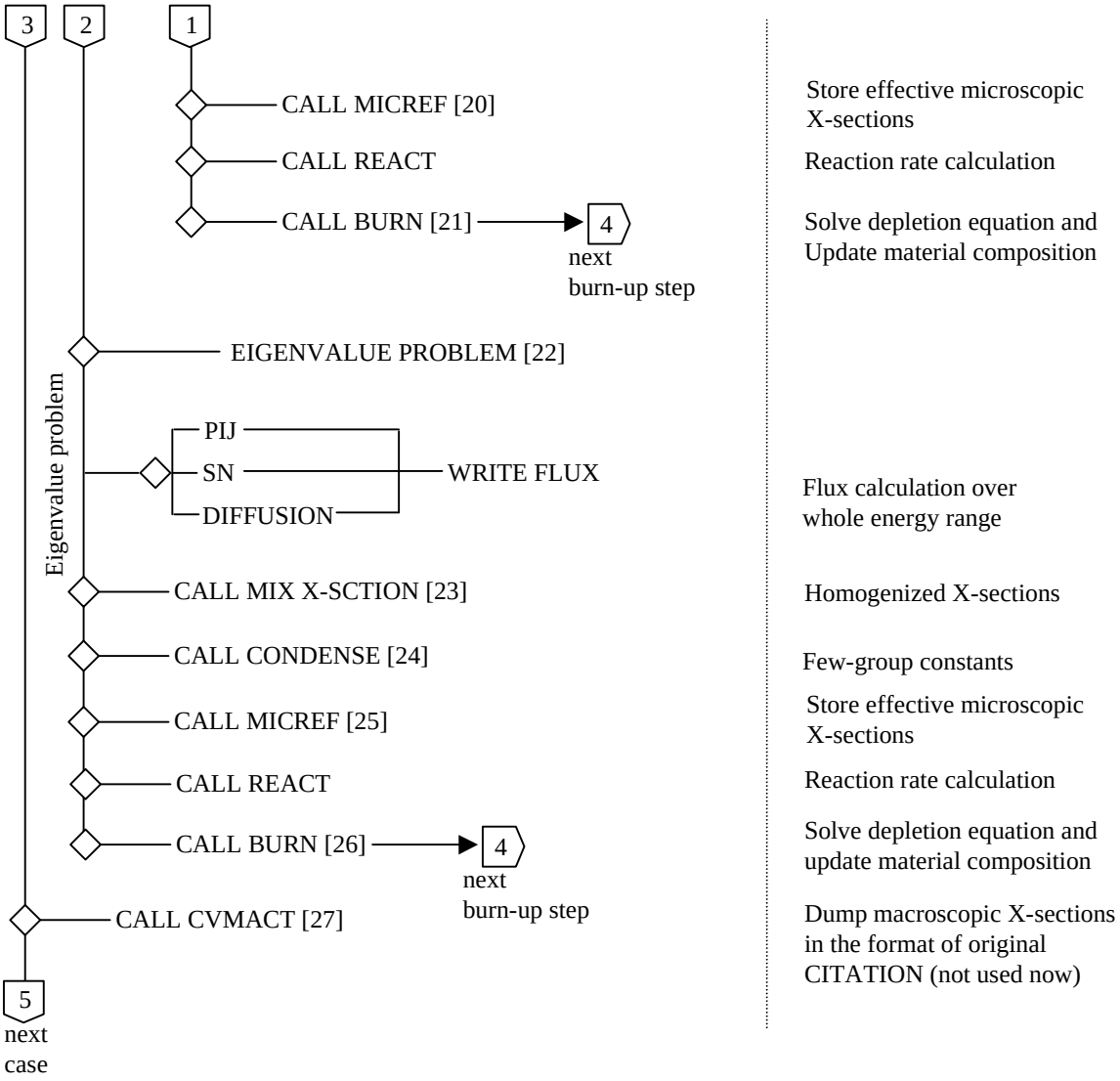


Fig.1.10-1 (2/2)　Flow daigram of the SRAC code

[Flow of the SRAC calculation for the sample problem]

UO2F ----------

READ CASE NAME

Read case name from the standard input in ‘A4’ format.

Some members to be stored in PDS files are named for this case name.

READ OPTION CONTROL

Read input data to control calculation flow. (cf. Sect.2.2 from Block-1 to -4)

READ FILE CONTROL

Read input data on PDS files and energy group structure.(cf. Sect.2.2, from Block-5 to -10)

PREPARE USER FAST AND THERMAL LIBRARY

Almost no action in this sample. (cf. Sect.2.3)

READ GEOMETRY FOR PIJ

Read input data for PIJ. (cf. Sect.2.4)

READ MATERIAL COMPOSITION

Read material specifications such as isotope composition and temperature. (cf. Sect.2.9)

COMPOSE USER LIBRARY

Compose the User Fast and Thermal Libraries by extracting and compiling the cross-section data of required nuclides from the Public Fast and Thermal Libraries. The 90-group cross-sections in the User Libraries are produced by collapsing 107-group ones in the Public Libraries with an asymptotic neutron spectrum (χ + 1/E + Maxwellian).

CALL MACRO-FAST

Compose effective microscopic and macroscopic cross-sections of each material in the fast energy range by the NR approximation, and store them in the MICREF and MACROWRK file, respectively.

CALL MACRO-THERMAL

Compose effective microscopic and macroscopic cross-sections of each material in the thermal energy range by the NR approximation, and store them in the MICREF and MACROWRK file, respectively.

CALL GAM

Form the macroscopic transport corrected cross-sections of each material. By choice of the option (IC16 in Sect.2.2), the P_1 or B_1 equation with an appropriate input buckling is solved for the cell homogenized by simple smearing of atomic number densities. Then, using the

homogenized P_1 spectrum obtained and assuming the flat flux, the transport correction is done for each material, and the MACROWRK file is updated.

FIXED SOURCE PROBLEM IN FAST

Enter into the process of the fixed source mode in the fast energy range

PIJ

Calculate collision probability in the fast energy range, then calculate fast neutron flux distribution on R-Region. The obtained flux is stored in the FLUX file.

CALL PEACO

Enter into the PEACO process

COMPOSE USER MCROSS LIB.

Compose the User MCROSS Library for the required nuclides and temperatures from the Public MCROSS Library.

HYPER-FINE FLUX CALCULATION

Calculate hyper-fine neutron spectra in the multi-region cell composed by R-Regions in the resonance energy range. Then, modify the effective absorption and fission cross-sections in MICREF and MACROWRK and the fine-group flux distribution in FLUX.

CALL MIX FAST X-SECTION

Homogenize the macroscopic cross-sections by X-Region

FIXED SOURCE PROBLEM IN THERMAL

Enter into the process of the fixed source mode in the thermal energy range

PIJ

Calculate collision probability in the thermal energy range, then calculate thermal neutron flux distribution on T-Region. The volume-averaged flux in each R-Region is stored in the FLUX file.

CALL MIX THERMAL X-SECTION

Homogenize the macroscopic cross-sections by X-Region

CALL HOMOSP

Solve a one-point (bare) reactor equation in whole energy range by P_1 or B_1 approximation with the input buckling to consider leakage effect. The k-infinity and k-effective together with the homogenized spectrum are obtained. The spectrum is stored in the FLUX file.

CALL CONDENSE

Condense the fine-group macroscopic cross-sections into few-group ones using the spectrum obtained by the above cell calculation. The few-group cross-sections are stored in the MACRO file.

Note: For the isolated material which does not appear in the cell, an asymptotic spectrum is used to condense the fine-group cross-sections. This treatment is used to make few-group cross-sections which is not so important for the core calculation. (e.g. radial water reflector). Otherwise, an appropriate cell or core calculation including the material have to be done to prepare a fine-group spectrum.

CALL MICREF

Print material-wise power distribution and conversion ratio

Note: The primary function of MICREF is to write the effective microscopic cross-sections in a scratch file for the succeeding reaction rate or burn-up calculation options.

MOXF ----------

READ CASE NAME

Read case name from the standard input in ‘A4’ format.

READ OPTION CONTROL

Read input data to control calculation flow.

READ GEOMETRY FOR PIJ

Read input data for PIJ.

:

the same as above case

:

CORE ----------

READ CASE NAME

Read case name from the standard input in ’A4’ format.

READ OPTION CONTROL

Read input data to control calculation flow.

READ GEOMETRY FOR DIFFUSION

Read input data for CITATION. (cf. Sect.2.8)

READ MATERIAL COMPOSITION

Read material specifications.

COMPOSE USER LIBRARY

Compose the User Fast and Thermal Libraries

Note: No action in this sample because of no new nuclides in the material specifications.

CALL MACRO-FAST

Compose effective microscopic and macroscopic cross-sections

Note: No action in this sample, because of no new nuclides in the material specifications.

Consequently next step 'CALL MACRO-THERMAL' is skipped.

CALL GAM

Form the macroscopic transport corrected cross-sections

Note : No action in this sample because of no new nuclides in the material specifications.

EIGENVALUE PROBLEM

Enter into the process of the eigenvalue mode

DIFFUSION(CITATION)

Compute k-effective and flux distribution by the whole energy calculation.

In this sample, CITATION is executed with few-group macroscopic cross-sections in the MACRO file by the choice of IC12=5 and IC10=1 (cf. Sect.2.2).

Note: As well as an eigenvalue calculation, an extra-source problem of CITATION (or other codes) is treated in this step.

READ CASE NAME

Read case name from the standard input in 'A4' format.

Terminate job by the specification of a blank case name.

Figure 1.10-2 shows the input data corresponding to the above sample problem, although details are omitted to emphasize the input data structure. As mentioned above, the first case (case name UO2F) requires to calculate the fine-group spectrum of the UO_2 cell by using PIJ and to obtain the homogenized and collapsed few-group cross-sections. The second case (MOXF) requires the same process as the first case for the MOX cell. The third case (case name CORE) requires a two-dimensional full core calculation by CITATION by using the few-group cross-sections provided by the first and second cases to yield the effective multiplication factor and the flux (or power) distribution. The cases can be repeated as far as the computation cost allows.

In this problem, the homogenized collapsed cross-sections are written in the few-group macroscopic cross-section file (MACRO) by the member names UO2FA010 and MOXFA010. The member name consists of the first four characters for the case name, the energy range by the fifth character, the burn-up step number by the sixth character, the homogenized region number by the seventh character and the group structure whether fine-group or few-group by the eighth character. The material specifications for the third case can be specified by only the names of members produced in the first and second cases. The PDS files take a role of an interface among the codes in the SRAC system.

```
UO2F  ← Case name for UO2 cell calculation
Macro-XS for UO2 CELL BY PIJ  ← Comment for this case
1 1 1 1 2   1 4 3 -2 1   0 0 0 0 2   0 1 0 0 0  ← Option control
1.0E-3 / BUCKLING FOR P1/B1
/home/okumura/SRACLIB-JDL33/pds/pfast      Old       File
/home/okumura/SRACLIB-JDL33/pds/pthml      O         F
/home/okumura/SRACLIB-JDL33/pds/pmcrs      O         F
/home/okumura/MyPDS/UFAST                  Scratch   Core
/home/okumura/MyPDS/UTHERMAL               S         C
/home/okumura/MyPDS/UMCROSS                S         C
/home/okumura/MyPDS/MACROWRK               S         C
/home/okumura/MyPDS/MACRO                  New       C
/home/okumura/MyPDS/FLUX                   New       C
/home/okumura/MyPDS/MICREF                 S         C
                                                          } PDS file control (first case only)
60 30   3 1 / Fast(60g)+Thermal(30g) => Fast(3G)+Thermal(1G)
          :
          :     { Energy Group Structure }
          :
          :     { Geometry for PIJ }
          :
3 / Number of Materials
FUE1X01X  0 3  300.  0.84  0.0  / 1 : UO2 FUEL
XU050001  2 0  6.086E-4
XU080001  2 0  2.255E-2
XO060001  0 0  4.725E-2
CLADX02X  0 1  300.  0.11  0.0  / 2 : CLADDING
XZRN0001  0 0  4.311E-2
MODEX031  0 2  300.  0.00  0.0  / 3 : MODERATOR
XH01H001  0 0  6.676E-2
XO060001  0 0  3.338E-2
                                                          } material specification
          :
          :
MOXF  ← Case name for MOX cell calculation
Macro-XS for MOX CELL BY PIJ  ← Comment for this case
1 1 1 1 2   1 4 3 -2 1   0 0 0 0 2   0 1 0 0 0  ← Option control
1.0E-3 / BUCKLING FOR P1/B1
          :
          :     { Geometry for PIJ }
          :
          :     { material specification for MOX fuel }
          :
CORE  ← Case name for Core calculation
2-dimensional Core calculation by CITATION (4-group)  ← Comment for this case
0 0 0 1 0   0 0 0 0 1   0 5 0 0 2   0 1 0 0 0  ← Option control
1.0E-20 / dummy BUCKLING (not effective)
          :
          :
          :     { Control and Geometry data for CITATION }
          :
005
  1  1  1
  1  2  1   ← Zone map
  1  1  1
          :
999

1 2  /  Material No. by Zone
2    / Number of Materials
UO2FA010 0  0  0.  0.  /  ← Homogenized X-section provided by the first case
MOXFA010 0  0  0.  0.  /  ← Homogenized X-section provided by the second case
     / End job  ← Blank case name to terminate job
                                                          } Input for CITATION
```

Fig.1.10-2 Sample input data structure of the SRAC code

1.11 Output Information

Major calculated results of the SRAC code are edited on a text-formatted file allocated to the 99th logical device. On the standard output file of the 6th device, information is written to check whether a series of calculations has completed appropriately or not, for instance, echo of user's input, status of calculation progress, record of PDS file access, warning or error message. When the calculation finished normally, the following message will be appeared at the last of the above two files.

```
'============================== END OF SRAC CALCULATION ======================='
```

Otherwise, a user has to check the standard output carefully.

For PIJ or PEACO, plotting options are available to confirm cell geometry under consideration or to draw hyper-fine neutron spectra obtained by PEACO. The plot data is written as a text-formatted Postscript file allocated to the 89th device. The user can see the figures of a Postscript file on a screen or printed matter, by using a free software on the market. On the UNIX operating system, a command 'lpr' is usually available to print out the figures.

In the case of the burn-up calculation, editing of the calculated results in each burn-up step is repeated up to the final burn-up step on the 99th file. Its contents may be enormous to extract necessary data. Therefore, major burn-up parameters are summarized and tabulated to the burn-up step on the 98th text-formatted file.

The binary data of fluxes and effective microscopic or macroscopic cross-sections are written in their own PDS files (cf. Sect.3.1). Although some of them can be printed on the 99th file by options, their printed format may not be convenient for plotting them or editing reaction rates defined by each user. In order to support editing or managing contents of PDS files, the SRAC system is equipped with several utility programs as described in Chapter 6.

2. Input Data Requirements

The input data requirements of the SRAC code consist of the following eleven input sections for a calculation case (cf. Sect. 1.10) in a job.

- General control and specification of group structure (always required)
- Specification of User library (always required)
- PIJ: Collision probability calculation
- ANISN: one-dimensional SN transport calculation
- TWOTRAN: two-dimensional SN transport calculation
- TUD: one-dimensional diffusion calculation
- CITATION: multi-dimensional diffusion calculation
- Material specification (always required)
- Reaction rate calculation
- Cell burn-up calculation
- PEACO: hyperfine resonance calculation

First elementary codes and functions to be used in a case are specified. After that, detailed input data for each code or function are specified if necessary. For a job with multiple-cases, a set of the above input sections are repeated necessary times.

2.1 SRAC Free Format

All input data for the SRAC system except for CITATION are read in a free format peculiar to SRAC. The features and usage are as follows.

(1) Three types of data array (character string of four bytes, integer, and floating point number of single precision) can be read.

e.g. TEST 1 2 1.00 2.00 3.00

(2) Columns 1 to 72 of a line record is used as data field. Data out of the field is neglected.

(3) A word (integer or floating number) is separated by a blank, a comma, or sign codes ‘+’ or ‘-‘ from the next word.

e.g. 1,2 3+4-5 is accepted as 1 2 3 4 -5

(4) A floating number may be entered by *F*-type or *E*-type; the latter needs the exponent code ‘E’ or ‘e’ at the beginning of exponent. *D*-type is not accepted.

e.g. -12.543 00.00125 1.0E-4 -.4E12 2.9e-2

(5) A word must be completed in a line record.

A wrong example: -12.543 0.00125 1.0E
-4 -.4E12

(6) Any blank column should not be inserted between sign code and digit code.

A wrong example: 1 2 - 3 4 - 5

(7) For *E*-type, any blank column should not be inserted between the exponent code ‘E’ or ‘e’ and the succeeding character.

A wrong example: 1.000E -5

(8) For character type, the style for the free format is not applied. Column position of character type variables is, in general, organized to start at the first column of a line record.

A wrong example: ABCD EFGH 4(IJKL)

(9) Repetition function is available. An integer before the code ‘(‘ is taken as the repetition number of a data or a series of data which are enclosed by ‘( )’.

e.g. 1 3(2) 2 (1.E-4) is accepted as 1 2 2 2 1.0E-04 1.0E-04

The data string enclosed by ‘( )’ can be written on more than one records. The closing ‘) ‘ may not be written on the first column.

e.g. 10 (1 2 3 4 5 4 3 2 1
5 4 3 2 1 2 3 4 5)

A wrong example: 2 (1 2 3 4
) 5 6 7 8

The duplicate use of ‘( )’ like 2(1 2(3 4)) is not allowed.

(10) Accumulation function is also available. An integer before ‘ * ‘ is taken as the number of times of accumulation, and the data value after ’ * ‘ is taken as increment to be added to the previous data. That is to say, ‘a b*c’ means ‘a a+c a+2c a+3c ..... a+bc’.

e.g. 0.0 4*1.0 2*-2.0 is accepted as 0.0 1.0 2.0 3.0 4.0 2.0 0.0

The coupling of ‘ ( )’ and ‘ * ‘ is not allowed.

A wrong example: 10(0 5*1)

(11) A series of strings for repetition or accumulation function must close within each type of array.

A wrong example: 10(1 1.0E-4)

(12) The character ' / ' is taken as the termination code of required data. The ' / ' is not necessarily required. If the termination code character is encountered, a check whether or not the array length

meets with one required by the program. However the character ‘ / ‘ on the new record after entering required data on the previous record causes error because the read-in is finished on the previous record without the termination code, then the code ‘ / ‘ is read at the beginning of the next call. The columns after ‘ / ‘ can be used as comment.

e.g. 5(0) 5(1) / Input data for Block-1

(13) The character ‘&’ is taken as the end-of-record code character. The columns after the ‘&’ can be used for comment. If the entries are not yet finished at this code, the remaining data follow on the next record.

An example when ten integers are required:

```
1  2  3  4  5  &  Input for Block-1(1-5)
& Comment 1
& Comment 2
6  7  8  9  10  /  End of Block-1
```

Although data type (character, integer or floating) of variable or array in the following description is not always mentioned, the user can recognize character type data by finding Hollerith count before the variable name as ‘/A8/’. Concerning to numerical data, the user can discriminate integer type or floating type by the first character of the variable name whether it is one of characters from I to N or not.

The term Block appearing in the descriptions denotes one or a series of data required by one FORTRAN read statement which may be entered on any number of lines. The use of the termination code ’ / ‘ is recommended to have suitable message if the data length is mismatched. The number of data required in a Block is shown as /20/ or /NRR/. If mixed types of data are required in a Block, they are read in the order of character, integer, then floating type, and the data requirement is expressed by /A8,3,2/ for 8 characters, 3 integers and 2 floating numbers, respectively.

2.2 General Control and Energy Structure Specification

Block-1 /A4/

CASENAME Case identification (*case*-tag)

It is used as the former half names of the members in the PDS files which store the macroscopic cross-sections (MACRO or MACROWRK) and fluxes (FLUX) homogenized in the X-Region.

As plural cases can be run in one job, enter a blank line after the last case to terminate the job.

[cf.] Sect.1.10, Sect.3.1

Block-2 Case description /A72/

TITLE Comments for the problem

Block-3 Integers to specify the options to control calculation flow /20/

IC1 Indicator to use the collision probability method routine (CPM) in any usage.

= 0 Skip

= 1 Use CPM

Note:

Enter IC1=1, if Dancoff correction factor is calculated automatically by CPM (IC3=1,2), or if PIJ is used for flux calculation (IC2=1, or IC12=±1), or if the PEACO routine is used (IC5=±2)

IC2 Selection of the routine for the fixed source mode (cf. Sect.1.7)

The problem is solved first in fast energy range where a uniform thermal flux distribution is assumed for providing the fast neutron source, then in thermal range.

= 0 None of routines is used. (Specify the routine for the eigenvalue mode by IC12.)

= 1 PIJ (CPM)

= 2 ANISN (one-dimensional S_N transport)

= 3 TWOTRAN (two-dimensional S_N transport)

= 4 TUD (one-dimensional diffusion)

= 5 CITATION (multi-dimensional diffusion)

Note:

Either IC2 or IC12 must be non-zero value. Enter IC2=0 and select the routine

by IC12, if the eigenvalue problem or the external neutron source problem in the whole energy range is solved. (e.g. shell source or distributed source in ANISN, inhomogeneous source or boundary source in TWOTRAN, point source in CITATION)

Enter IC2=1 if the PEACO routine is used by IC5=2 or =-2 for the resonance absorption process.

[cf.] Sect.1.7, Sect.1.10

IC3 Selection of the process to get the Dancoff correction factor

The Dancoff correction factor is used in the two steps; first for the heterogeneous effect on the admixture cross-sections in the interpolation of resonance shielding factors upon NR approximation, second for the IR approximation of absorption calculations of resolved resonance levels.

= 0 Use the input value specified in the material specification (cf. Sect.2.9)

= 1 Calculate by CPM

= 2 Calculate by the Tone's method[12)]

Note:

The Tone's method is recommended for a plate type cell with neighboring different fuels, but it is not recommended for a pin type cell.

When the double heterogeneity is solved by the PEACO routine by specifying a negative value of MAR (Block-6 in Sect. 2.4), the Dancoff correction factor of the microscopic heterogeneity in the material specification is used in spite of any IC3 value while that of the macroscopic heterogeneity is controlled by the IC3 value.

[cf.] Sect.1.6, Sect.2.4

IC4 Indicator for the energy range solved

= 0 Thermal range is excluded (for fast neutron reactors)

= 1 Thermal range is included (for thermal neutron reactors)

IC5 Selection of the process for resonance absorption in the resonance energy range

= 0 Interpolation of Bondarenko type table by NR approximation(NRA).

= 1 Interpolation of Bondarenko type table by IR approximation (IRA).
The IRA routine works for only one resonant R-Region (which contains at least one nuclide(s) with IRES=2 in the material specification) in a

cell.

= 2 The PEACO routine (hyperfine group calculation by the CPM)
The PEACO routine runs only on the fixed source mode by PIJ (IC2=1).
The number of resonant materials (which contains at least one nuclide(s) with the MCROSS library data) is limited one or two.

= -2 The PEACO routine to treat more than two resonant materials by an approximation to assume two pseudo resonant materials.
Additional input (in Sect.2.12) is required to assign the materials to which resonant material belongs.

Note:

The PEACO routine generally does not work for more than two resonant mixtures in a cell because the two-dimensional interpolation of collision probabilities is done for completely different resonant materials. When a depletion problem is solved for a multi-region cell, several compositions which have been uniform at the clean stage have to be considered in a cell. The similarity of cross-sections can permit the above-mentioned approximation.

[cf.] Sect.1.5, Sect.1.6, Sect.2.12

IC6 Indicator to get the flux-volume averaged cross-sections in the fixed source mode (IC2>0). Enter 0 in the eigenvalue mode.

= 0 Skip the averaging process

= 1 Call the averaging process specified by IC7 following

IC7 Selection of the process to get the spatial distribution of flux in each energy range.

= 0 for the eigenvalue problem mode (IC2=0, IC12 $\neq$ 0)

= 4 for the fixed source problem mode (IC2>0, IC12=0)

Note:

This option was originally prepared for computer time saving by skipping (if IC7=1~3) the calculation of spatially flat and nearly asymptotic neutron spectrum foreseen by the user in the fixed source problem. Enter IC7=4 in the fixed source problem. Otherwise enter IC7=0, because the other selections (IC7=1~3) are obsolete and not recommended.

IC8 Selection of the energy range and mesh of the hyperfine group structure of the

user's MCROSS library, required if the PEACO routine is used by IC5=±2. The selection IC8=3 is usually recommended.

= 0 between 130.07 eV and the thermal-cut-off energy with lethargy interval of Δu=0.00125

= 1 between 130.07 eV and the thermal-cut-off energy with lethargy interval of Δu=0.00125 and between 961.12 eV and 130.07 eV with lethargy interval of Δu=0.000625

= 2 between 961.12 eV and the thermal-cut-off energy with uniform lethargy interval of Δu=0.0005

= 3 between 130.07 eV and the thermal-cut-off energy with lethargy interval of Δu=0.0005 and between 961.12 eV and 130.07 eV with lethargy interval of Δu=0.00025

[cf.] Sect.1.3, Sect.1.6, Sect.1.10

IC9 Indicator to call the HOMOSP routine to calculate the one point (bare) reactor neutron spectrum and k_∞, k_{eff} in the fixed source problem (IC2>0). Enter IC9=0 in the eigenvalue problem mode.

= 0 Skip

= ±1 P_1 approximation

= ±2 B_1 approximation

= ±11 Critical buckling search by P_1 approximation

= ±12 Critical buckling search by B_1 approximation

Note:

If negative value is entered, P_0 components of the solution of P_1 or B_1 equations are used as the weight to collapse the homogenized cross-sections, i.e. the leakage effect is reflected on the spectrum by the geometrical buckling value. If positive value is entered, the spectrum obtained by the cell calculation is used for collapsing.

The CPM is carried out upon infinite cell approximation. The geometrical buckling is used to reflect the leakage effect on the spectrum by use of the HOMOSP routine.

If IC9=±1 or =±2 is entered, the geometrical buckling given in Block-4 is used in P_1/B_1 equations. If IC9=±11 or =±12 is entered, the geometrical buckling is obtained so that the k_{eff} is unity. The use of the critical buckling search option

should be avoided for the core where the large excess reactivity is mainly suppressed by using control absorber.

[cf.] Sect.1.7, Sect.1.10

IC10 Indicator to call CONDENSE routine to collapse the energy structure of the macroscopic cross-sections in the MACROWRK file to put into the MACRO file before the eigenvalue mode calculation specified by IC12.

= 0 Skip the collapsing

= 1 Collapse before the eigenvalue mode calculation (if any)

Note:

If the user wants to execute the fixed source mode by the routine specified by IC2 on the fine-group and then the eigenvalue problem by the routine specified by IC12 on the collapsed group structure, enter IC10=1, IC13=0 for the first case, and enter also IC10=1, IC13=0 for the second case.

If the user wants to execute a cell calculation by the fixed source mode on the fine-group structure to provide the fine-group homogenized cross-sections, and then to execute a super-cell calculation on the fine-group structure to provide the collapsed group cross-sections for the succeeding core calculation, enter IC10=0, IC13=1 in the first case, and IC10=1, IC13=0 for the second case.

Thus, if the collapsing is required in a job, any of IC10 or IC13 must be 1 at the first case. The entries IC10=1 and IC13=1 in a case are not accepted.

IC11 Indicator whether to enter or not the geometrical information required in Sect. 2.4 through 2.7 for this case.

= 0 Read the new geometry.

= 1 Skip reading and use the same as the previous case. Ineffective for CITATION.

IC12 Selection of the routine for the eigenvalue mode (whole energy range calculation).

= 0 None of routines is used. (Specify the routine for the separate energy calculation by IC2.)

= ± 1 PIJ (CPM)

= ± 2 ANISN (one-dimensional S_N)

= 3 TWOTRAN (two-dimensional S_N)

= 4 TUD (one-dimensional diffusion)

= 5 CITATION (multi-dimensional diffusion)

Note:

If IC12=-1 is entered, the incident current at the outer boundary is read from the FLUX file by the member *case*A*b*S*p* (cf. Sect.3.1.7) so that a fixed boundary source problem in the whole energy group will be solved.

If IC12=-2 is entered, the collapsing of P_1 components is carried out for the succeeding few-group transport calculation. (See IC16)

[cf.] Sect.1.7, Sect.1.10

IC13 Indicator whether or not to call CONDENSE to collapse the energy group structure of the macroscopic cross-sections in the MAROWRK file to put into the MACRO file after the eigenvalue mode calculation specified by IC12.

= 0 Skip the collapsing

= 1 Collapse after the eigenvalue mode calculation (if any)

Note:

For example, to execute an eigenvalue calculation by using the cross-sections of the fine-group structure stored in the MACROWRK file and to obtain the few-group cross-sections by using the flux solved by the above calculation, enter IC10=0, IC13=1.

[cf.] Sect.1.7, Sect.1.10, IC10 in this Section

IC14 = 0 (not used)

IC15 Selection of the process to compose (or define) the microscopic total cross-sections in the resonance energy range. (out of energy range of PEACO, if IC5=2 or -2)

= 1 Form the cross-sections by using the self-shielding factor of the total cross-sections. The in-group scattering cross-sections are adjusted to hold the neutron balance.

$$\sigma_{t,g} = \sigma^{\infty}_{t,g} f_{t,g}$$

= 2 Form the cross-sections by summation of all partial reactions

$$\sigma_{t,g} = \sum_{x} \sigma^{\infty}_{x,g} f_{x,g}$$

Note:

Usually IC15=1 is used in FBR analysis, while any selection does not make difference in thermal reactor analysis.

IC16 Indicator how to form the macroscopic transport (collision) cross-sections of each mixture which are required in the isotropic transport routine.

= 0 The extended transport approximation[23)]

$$\Sigma_{tr,g} = \Sigma_{0,g} - \sum_{g'} \Sigma_{1,g'\to g}$$

However, in the resonance shielding calculation $\Sigma_{tr,g}=\Sigma_{0,g}$ is always assumed.

= 1 Use the components (J) obtained by the P_1 approximation[24)]

$$\Sigma_{tr,g} = \Sigma_{0,g} - \sum_{g'} \Sigma_{1,g'\to g} J_{g'} / J_g$$

= 2 Use the current component (J) obtained by the B_1 approximation[24)]

$$\Sigma_{tr,g} = \Sigma_{0,g} - \sum_{g'} \Sigma_{1,g'\to g} J_{g'} / J_g$$

= 3 Use the current component (P_1 flux) obtained by the ANISN calculation

$$\Sigma_{tr,g} = \Sigma_{0,g} - \sum_{g'} \Sigma_{1,g'\to g} J_{g'} / J_g$$

An ANISN calculation in the fine-group structure is required in the previous case with IC12=-2 so that the corresponding members have to be stored in the FLUX file.

Note:

For the fixed source mode (IC2>0), a fixed source problem by one-point fine-group equations with P_1 or B_1 approximation selected is solved for an imaginary media made by the homogenized cross-sections averaged in the whole system where a flat flux approximation and the fission spectrum of U-235 are assumed.

For the eigenvalue mode (IC2=0 and IC12>0), a fixed source problem is solved to obtain the current components at each constituent material. In the above equations, the geometrical buckling given in Block-4 is used in the leakage term, and the source is assumed to be same as the fission neutron spectrum of U-235.

When the P_1 or B_1 option is used for a material which is a strong absorber such as a control rod material or a highly enriched plutonium, or an optically transparent

material such as an aluminum metal, the iterative process to obtain the spectrum may fail to converge.
[cf.] Sect.1.10

IC17 Indicator how to compose and to collapse the averaged diffusion coefficients

The absolute value of this item defines the way of spatial average of the diffusion coefficients in the fine-energy group stage, and the sign of IC17 defines how to collapse the diffusion coefficients and the total (transport) cross-sections into the few group constants.

If IC17>0

$$D_G = \sum_{g\in G} D_g \varphi_g \,/\, \sum_{g\in G} \varphi_g \quad , \quad \frac{1}{\Sigma_{t,G}} = \sum_{g\in G} \frac{1}{\Sigma_{t,g}} \varphi_g \,/\, \sum_{g\in G} \varphi_g$$

If IC17<0

$$\Sigma_{t,G} = \sum_{g\in G} \Sigma_{t,g} \varphi_g \,/\, \sum_{g\in G} \varphi_g \quad , \quad D_G = \sum_{g\in G} D_g \varphi_g \,/\, \sum_{g\in G} \varphi_g$$

It is recommended that for the succeeding diffusion calculation, enter positive value, and for the succeeding transport calculation enter negative value.

Note that only in case of IC17=±1, the few-group diffusion coefficients are made from the inverse of the few-group transport cross-sections as $D_G = 1/3\Sigma_{tr,G}$.

After obtaining the few-group total cross-sections, the self-scattering (in-group scattering) cross-sections are adjusted to keep the neutron balance.

Two kinds of diffusion coefficients D1 and D2 are stored in the MACRO and the MACROWRK files to allow a CITATION calculation with direction dependent diffusion coefficient.

= ±1 The fine group diffusion coefficients are made from the inverse of the fine group transport cross-sections.

$$D_g = 1/3\Sigma_{tr,g}$$

The calculated values are stored in the D1 position. (cf. Sect.3.1)

= ±2 The diffusion coefficients are formed by the isotropic components of

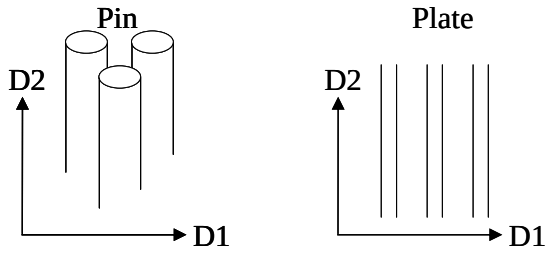
Behrens' term of the Benoist model[25] which are written into D1 positions in the MACROWRK file.

$$D_g = \left\{ \sum_i \varphi_{i,g} \sum_j P_{i->j,g} / \Sigma_{tr,j,g} \right\} / 3 \sum_i \varphi_{i,g}$$

= ±3 The anisotropic components of the Behrens' term of the Benoist model.

$$D_{k,g} = \left\{ \sum_i \varphi_{i,g} \sum_j P_{i->j,k,g} / \Sigma_{tr,j,g} \right\} / 3 \sum_i \varphi_{i,g}$$

The radial components in the cylindrical coordinate or the perpendicular components in the plate geometry are written into D1, and the axial components in the cylindrical or the parallel components in the plate are written into the D2 position.



Note:

Unless IC17=±3, the values stored in D2 position are made as if the options IC16=0 and IC17=1 are specified.

IC18 Indicator to call the reaction rate calculation.

= 0 Skip

= 1 Call reaction routine.

The input described in Sect.2.10 is required.

IC19 Print control in the routines for forming the macroscopic cross-sections (MACROF, MACROT, P1B1, HOMOSP, IRA, PEACO)

= 0 The most brief edit

> 0 The larger value prints the more fine information, (usually up to 2)

IC20 Indicator to call the cell burn-up calculation

= 0 Skip

= 1 Execute burn-up calculation

Note:

If the system contains a homogenized region which occurs in a super-cell calculation, the cell burn-up calculation is not available.

[cf.] Sect.1.9

Block-4 Geometrical buckling B^2 (cm^{-2}) /1/

BSQ Buckling value commonly used in the P_1 or B_1 approximation in one-point reactor calculation specified by IC9 (HOMOSP routine) and/or IC16 (GAM routine).

The negative value is accepted while zero value is rejected. Set a value about 1.0E-20 instead of 0.0, as an extremely small value less than 1.0E-20 may cause a numerical overflow.

Even if the buckling search is specified by IC9, the input value is used in the process specified by IC16.

<u>The succeeding input Block-5 through Block-10 are required only in the first case.</u>

Block-5 Data set specification for PDS files /A72/

One file is specified by PATHNAM, KPMODE, IOMODE on 72 columns. They are separated by one or more blank(s). This type input must be repeated 10 times : the total number of PDS files in the order of 1)PFAST, 2)PTHERMAL, 3)PMCROSS, 4)UFAST, 5)UTHERMAL, 6)UMCROSS, 7)MACROWRK, 8)MACRO, 9)FLUX and 10)MICREF files.

PATHNAM(*i*) path name to a PDS file

Specify the directory in which members are stored by the absolute path or by the relative path. Enter from the 1st column.

An example of an absolute path:

/home/okumura/SRACLIB-JDL33/pds/pfast

An example of a relative path:

../../SRACLIB-JDL33/pds/pfast

KPMODE(*i*) the preservation mode of a PDS file

Only the first character (capital letter) is effective.

=New New file, there is no practical difference with old file.

=Old Old file

=Scratch Scratch file, ineffective for the Public Libraries (read only files)

Note:

When ’New’ or ‘Old’ is specified, all the members produced are preserved after the job. If ’Scratch’ is specified, the members are deleted.

The preservation or deletion of the PDS directory is controlled by the description of shell-script. Even if ‘Scratch’ is specified here, an empty directory remains when the directory is not deleted by the shell-script. The ’New’ specification requires that the directory of the same name of PATHNAM should be prepared by shell-script beforehand.

IOMODE(*i*) Access mode to file

Only the first character (capital letter) is effective.

=File Direct I/O access to file

=Core I/O access on image PDS file on core memory

Note:

If ‘Core’ is specified, all the information on a PDS file is read into the core memory at the first access. After this, I/O is carried out from/into the core. A new member is also written on the actual file.

When the overflow of memory occurs on any PDS file, the Core specifications to all the PDS files are switched to File mode automatically. The core specification is effective for the job which takes much I/O time.

The IOMODE specifications to the Public Library files are compulsorily set to ‘File’ mode as they are used only to make User’s Library files and a large amount of data is stored.

When a series of burn-up calculation is executed, as a lot of members are written, a sufficient amount of memory has to be reserved. The memory capacity for PDS files is defined by a parameter statement in an include file.

An example of Block-5 input:

```
/home/okumura/SRACLIB-JDL33/pds/pfast      Old     File
/home/okumura/SRACLIB-JDL33/pds/pthml      O       F
```

```
/home/okumura/SRACLIB-JDL33/pds/pmcrs      O       F
/home/okumura/MyPDS/Test/UFAST             Scratch Core
/home/okumura/MyPDS/Test/UTHERMAL          S       C
/home/okumura/MyPDS/Test/UMCROSS           S       C
/home/okumura/MyPDS/Test/MACROWRK          S       C
/home/okumura/MyPDS/Test/MACRO             New     C
/home/okumura/MyPDS/Test/FLUX              New     C
/home/okumura/MyPDS/Test/MICREF            S       C
```

Block-6 Specification for energy group structures /4/

1 NEF Number of the fast neutron groups of the User Fast Library (NEF $\leq$ 74)

2 NET Number of the thermal neutron groups of the User Thermal Library;
(NET $\leq$ 48, and NEF+NET $\leq$ 107).
Enter 0, if IC4 = 0 (no thermal group calculation) in Block-3

3 NERF Number of the fast few-groups
If no collapsing is required (IC10=0 and IC13=0), enter NERF=0.

4 NERT Number of the thermal few-groups
If no collapsing is required (IC10=0 and IC13=0) or no thermal group calculation (IC4=0), enter NERT=0.

Block-7 Collapsing from PFAST into UFAST /NEF/

NEGF(i) Number of the public fast groups in each user fast group (i)
See the table of energy group structure in Sect. 8.3.

$\sum_{i=1}^{\mathrm{NEF}} \mathrm{NEGF}(i)$ =(Total number of public fast groups included between 10 MeV and the thermal-cut-off energy). By this item, the thermal-cut-off energy is decided.

As the thermal-cut-off energy has to be any of lower energy boundaries of Public energy group structure between 3.9278 eV and 0.41399 eV, set NEGFs so as to satisfy $59 \leq \sum_{i=1}^{\mathrm{NEF}} \mathrm{NEGF}(i) \leq 74$.

The recommended cut-off-energy in the SRAC code is about 2.0 eV (cf. Sect.1.3)

Block-8 Collapsing from PTHERMAL into UTHERMAL, Required if NET $\neq 0$ /NET/

NEGT(i) Number of the public thermal groups in each user thermal group (i)
See the table of energy group structure in Sect. 8.3.

$\sum_{i=1}^{NET}$ NEGT(i) =(Total number of public thermal groups below the thermal-cut-off energy).

The relation $\sum_{i=1}^{NEF}$ NEGF(i) + $\sum_{i=1}^{NET}$ NEGT(i) = 107 must be satisfied.

Block-9 Required if NERF $\neq 0$ is specified /NERF/

NECF(i) Number of the user fast groups in each condensed fast group (i)

The relation $\sum_{i=1}^{NERF}$ NECF(i) = NEF must be satisfied.

Block10 Required if NERT $\neq 0$ is specified /NERT/

NECT(i) Number of the user thermal groups in each condensed thermal group (i)

The relation $\sum_{i=1}^{NERT}$ NECT(i) = NET must be satisfied.

An example of the Block-6 through Block-10

```
-------------------------------------------------------------------------------------------------------
62 45  2 1     /  107(=62+45) fine-group => 3(=2+1) few-group
62(1)          /  No collapsing from PFAST to UFAST (cut-off=1.85eV)
45(1)          /  No collapsing from PTHERM to UTHERM
28 34          /  Block-9
45             /  Block-10
-------------------------------------------------------------------------------------------------------
```

2.3 User's Library Specification

Formally all of the nuclides used in the succeeding calculations had to be specified in this section to transfer the necessary cross section data from the Public Library to User's Library. In the current version, the requirements are automatically judged from the material specifications in Sect.2.9 and the burn-up chain library in Sect.3.3. Thus, the user completes the section by feeding one blank line.

A special option is provided for the case where a job was terminated with the following error message:

```
 ------------------------------------------------------------------------------------------
 NUCLIDE(xxxxxxxx) HAS DOUBLE TEMPERATURE DEFINITION.
 ONE TEMPERATURE IS xxx.xx KELVIN AND ANOTHER IS yyy.yy KELVIN.
 PLEASE RESET STATNDARD TEMPERATURE ARRAY BY YOUR INPUT DATA
 ------------------------------------------------------------
```

This message appears when a resonant nuclide with the MCROSS library data is included in two or more mixtures of different temperatures, and the PEACO routine is used for the resonance absorption calculation. To avoid this, the following Blocks are required before a blank line.

Block-1	Keyword to call the input requirement	/A8/
NMTEMP	Enter 'TEMPSET '	
	Keyword to call input requirement	
Block-2	Required if Block-1 is specified	/35/
STND(*i*)	The temperatures (K) appearing in the material specifications in ascending order. Fill 0.0 for residual array of the input data.	

An example of Block-1 and Block-2 (bold parts):

```
------------------------------------------------------------------------------------------------------
62 45  2 1     /  Block-6 in Sect.2.2 (107 group => 3 group)
62(1)          /  No collapsing from PFAST to UFAST
45(1)          /  No collapsing from PTHERM to UTHERM
28 34          /
45             /
TEMPSET
581.  600.  900.  1000.0   31(0.0) / STNDTMP(35)
                                   ←( one blank line to terminate input of this section.)
4 6 6 4 1   1 6 0 0 0   5 0 6 15 0   0 45 0    / Pij Input
          :
          :
4 / Material Specification
FUE1X01X  0 3  1000.  0.557    0.0  / 1 : FUEL-1
XU050009  2 0  7.0908E-4       /1
XU080009  2 0  2.1179E-2       /2
XO060009  0 0  4.3777E-2       /3
FUE2X02X  0 3  900.   0.278    0.0  / 2 : FUEL-2
XU050009  2 0  7.0908E-4       /1
XU080009  2 0  2.1179E-2       /2
XO060009  0 0  4.3777E-2       /3
CLADX03X  0 1  600.   0.114    0.0  / 3 : CLADDING
XZRN0008  2 0  4.2507E-2       /1
MODEX04X  0 7  581.   1.000    0.0  / 4 : MODERATOR
XH01H008  0 0  4.5869E-2       /1
XO060008  0 0  2.2934E-2       /2
          :
------------------------------------------------------------------------------------------------------
```

2.4 PIJ ; Collision Probability Method (CPM)

The input of this section is required if IC1=1 and IC11=0 to specify the control variables, geometry model, computation accuracy, and options used in the calculation of collision probabilities.

Block-1 Control integers /18/

1 IGT Geometry type (See Fig.2.4-1 through 2.4-6)

= 1 One-dimensional sphere of multi-shells with the isotropically reflective condition at the outer boundary.

= 2 One-dimensional slab of multi-layers.

Care should be taken of the boundary condition. If IBOUND=1 is specified, not the perfect reflective (mirror) boundary condition but the periodic condition is applied for this geometry so as to treat an asymmetric cell. On the other hand, if a symmetric lattice is considered, the full geometry must be given.

= 3 One-dimensional circular cylindrical divided by concentric annuli.

= 4 Square cylinder divided by concentric annuli.

A square cell is divided by the concentric circles into several regions. It is to be noticed that the cell can be divided by the circle of which radius exceeds the distance from the center to the flat.

= 5 Square cylinder of two-dimensional division.

A square cell sub-divided by the concentric circles and further by four lines crossing the central axis. Each line makes an angle of 67.5° with a flat of the square. While an annular ring is divided into eight pieces, because of the octant symmetry assumed, two adjacent pieces per annular division are left as independent regions.

= 6 Hexagonal cylinder divided by concentric annuli.

= 7 Hexagonal cylinder of two-dimensional division.

A hexagonal cell is divided by the concentric circles and also by six lines crossing the central axis. Each line makes an angle of 75° with a flat of the hexagon. While an annular ring is divided into twelve pieces, because the 60° rotational symmetry is assumed, two adjacent pieces on an annular division remain as independent regions.

= 8 Octant symmetric square pillar divided by X-Y coordinates.

= 9 Octant symmetric square pillar divided by X-Y coordinates with square array of pin rods.

A pin rod can not lie on the grid line specified by RX(*i*). Different

radius by pin is accepted.

S-Regions are numbered by the rules 1) coolant regions ahead of pin rod regions, 2) lower to upper, 3) left to right, 4) inner to outer in a pin rod.

= 10 Annular assembly with annular array of pin rods.

A circular cylindrical assembly is divided by concentric annuli specified by RX(*i*). A certain number NPIN(*j*) of pin rods are placed on circular annuli specified by RPP(*j*). They must be placed with equal spacing on their azimuthal angles because the pin rods on a circle are assumed equivalent. A pin rod is sub-divided into several concentric layers by RDP. All the pin rods have the same geometry. The pin rods may, together with the coolant, be divided further radially into inner and outer by the circles denoted by RPP(*j*) by an option indicator IDIVP.

S-Region is numbered first to the inner-most pin rod starting from inner to outer of a pin rod if IDIVP<2, and from inner to outer measured from the cell center if IDIVP=2, then to the pin rod on the outer ring. After the outer-most pin rod, the coolant region follows from the inner to the outer.

Note that the cylindrical approximation is made for the outer boundary of a unit assembly.

= 11 Annular assembly with asymmetric array of pin rods.

The model IGT=10 is extended to permit an asymmetric disposition of pin rods. Any size of pin rod can be mounted at an arbitrary position as far as pin rods do not intersect each other. The coolant regions can be subdivided two-dimensionally by the concentric circles and by the radiating lines.

The numbering of S-Regions obeys principally the same rule as IGT=10. In view of azimuthal angle, the region positioned at smaller angle comes ahead.

Care should be taken in applying the isotropically reflective boundary condition at the outer surface where the neutron flux is assumed uniform and isotropic even if the fluxes in the segment regions adjacent to the surface are not uniform in the rotational direction. It is suggested to use this model in the so-called super-cell structure in which an actual

asymmetric cell is surrounded by enough thick symmetric material and the isotropic boundary condition is applied at the outer boundary of this external material.

= 12 Hexagonal assembly with asymmetric array of pin rods.

A model is provided to permit a hexagonal block with asymmetrical array of pin rods. Except the shape of the outer surface, the input requirements and the rule of S-Region numbering are same as those of IGT=11.

= 13 Rectangular pillar divided by X-Y coordinates with pin rods on grid points.

This type permits the placement of pin rods on any grid point of an X-Y division of a rectangular lattice cell. Every pin rod has its own radius with annular sub-division.

When IBOUND=1 is specified as the outer boundary condition, not the perfect reflective but the periodic condition is supposed in x- and y-direction. As S-Region numbers are purely geometrical, the user is requested to allocate T- and R-Region numbers so as to satisfy the periodic condition. For example, the region number allocated to a fuel pin located on the left edge must be coincide to that on the right edge.

S-Regions are numbered by the rules 1) coolant regions ahead of pin rod regions, 2) small Y-abscissa to large abscissa, 3) small X-abscissa to large abscissa, 4) inner to outer in a pin rod.

= 14 Concentric layer of hexagons with pin rod array of 60° symmetry.

A hexagonal assembly is divided by several concentric hexagons. On the flat of the arbitrary hexagon, pin rods of the uniform size can be mounted. Number of pin rods on a hexagon must be a multiple of six, since the 60° rotational symmetry is assumed. They are placed with equal interval starting at a corner of a hexagon. Pin rods on a hexagon are treated to have the same fluxes.

S-Regions are numbered by the rules 1) pin rod regions ahead of coolant regions, 2) inner to outer in an assembly, 3) inner to outer in a pin rod. But in case of IDIVP=2, pin rod regions are numbered by the distance from the central axis of the assembly.

= 15 Hexagonal assembly of 60° rotational symmetry with pin rods on

triangular grid points .

Difference from IGT=14 is that 1) coolant regions are divided by triangular meshes, 2) each pin rod can have the particular size, and 3). trapezoidal shape regions near the outer boundary of the assembly can simulate the wrapper tube and inter-assembly gap.

As the perfect reflective boundary condition is not supported, the isotropically reflective condition is applied.

S-Regions are numbered by the rules: 1) coolant regions ahead of pin rod regions. For coolant regions, 2.1) from inner to outer measured from the central axis, 2.2) small Y-abscissa to large Y-abscissa, For pin rod regions, 3.1) inner to outer in a pin rod, 3.2) small Y-abscissa to large Y-abscissa, 3.3) inner to outer measured from the central axis.

= 16 Rectangular pillar divided by X-Y coordinates of quadrant symmetry with pin rods on grid points.

This type permits the placement of pin rods on any grid point of an x-y division of a rectangular lattice cell. Every pin rod has its own radius with annular sub-division. This model differs from the model IGT=13 by applying the perfect reflective boundary conditions always on the left surface and on the lower surface.

When IBOUND=1 is specified as the outer boundary condition, the perfect reflective condition is applied on the right and the upper surfaces.

S-Regions are numbered by the rules 1) coolant regions ahead of pin rod regions, 2) small Y-abscissa to large abscissa, 3) small X-abscissa to large abscissa, 4) inner to outer in a pin rod.

2 NZ Total number of Sub-Regions

3 NR Total number of T-Regions

4 NRR Total number of R-Regions

5 NXR Total number of X-Regions

6 IBOUND Outer boundary condition of the cell calculation

= 0 Isotropic (white) reflection

= 1 Perfect reflection (mirror)

For IGT=2 (1D slab) or IGT=13 (2D X-Y pillar) periodic condition is applied. For IGT=15, IBOUND=1 is ineffective.

= 2 Isolated (black)

= -1 60° rotational (applicable only for IGT=12)

Note:

It is recommended that reflective boundary condition at the outer surface for sphere (IGT=1) or cylinder (IGT=3, 10, 11) should be not perfect but white reflection.

If the fixed boundary source problem is solved by the specification of IC12=-1, IBOUND is automatically set to black.

For the optically large assembly, IBOUND=0 is recommended to avoid much computation time.

7 NX Number of mesh intervals for X division (IGT=2,8,9,13,15,16)
Number of mesh intervals for R division (IGT=1,3,4,5,6,7,10,11,12,14)

8 NY Effective for IGT=11,12,13,15,16
Number of mesh intervals for Y division (IGT=13,16)
Number of mesh intervals for angular division (IGT=11,12)
Number of mesh intervals for the division along the flat of outer trapezoidal regions (IGT=15)

9 NTPIN Total number of pin rods (effective for IGT=10,11,12,13,14,15,16)
This item is calculated internally for IGT=9 by NAPIN.

For IGT=10,11,12, the pin rod on the central axis is not counted as a pin rod, then, the central pin has to be entered by RXs. For IGT=14,15, the pin rod on the central axis is counted as a pin rod. For IGT=15, although 60° rotational symmetry is assumed, enter total number of pin rods in an (6/6) assembly.

10 NAPIN Effective for IGT=9,10,14,15
Number of pin rods in an array on X-direction (for IGT=9).
Number of circles on which the pin rods are located (for IGT=10). The central axis

is not counted for NAPIN.

Number of hexagons on which the pin rods are located (for IGT=14). The central axis is counted for NAPIN.

Number of triangular meshes on X-axis (for IGT=15) where (NX-NAPIN) are number of layers of outer trapezoidal regions.

11 NCELL Minimum number of lattice cells traced by a neutron path

This item is effective only for IBOUND=1 for geometries of non-circular outer shape. This is used to cut off a neutron path without knowing the actual optical path length. It is desirable to trace a neutron beyond an optical length of 6.0 if the computer time allows. Recommended value to this item is NCELL=2 for a cell enough large in the sense of optical path, or NCELL=5 for a transparent or small cell. The larger value causes the longer computer time. The user should not be afraid of the short cut of a path by insufficient number of NCELL while a certain amount of neutrons reach the end of the path and loose the contribution. It will be recovered by the later process of normalization and redistribution of collision probabilities.

If the negative value is entered, the new algorithms for vectorized calculation for the numerical integration of collision probabilities is applied. As the computing time depends on the geometry and the boundary condition, the comparison of CPU time by both algorithms is recommended before repetitive calculation of same geometry.

12 IEDPIJ Edit control for collision probabilities

= 0 Skip print

= 1 Print collision probabilities

13 NGR Order of Gaussian integration for the numerical radial integration

This item is ineffective for one-dimensional slab (IGT=2). Recommended value is from 6 to 10. The computer time for the integration of collision probabilities is proportional to this item. For the geometries IGT=8,9,13,15 and 16 the Gaussian integration is replaced by the trapezoidal rule.

14 NDA Number of division of the range IBETM (described below) entered by the unit of

degree for the numerical angular integration of the collision probabilities.

Required for two-dimensional integration for IGT 4 through 16. Sufficient accuracy will be attained if approximately IBETM/2 is entered as NDA.

Total amount of NX*NGR*NDA neutron paths are traced for the two-dimensional integration. After storing the path information and before the actual time-consuming integration, the ratios of the numerically integrated volumes to the exact ones are printed out. The deviations of the ratios from unity (should be less than a few percent) predict the accuracy of the integration. The user should adjust the values of NGR and NDA so as to be accurate but not time-consuming.

15 NDPIN Number of annular division of a pin rod (effective for IGT=9 through 16)

16 IDIVP Control of sub-division by RPP (effective for IGT= 9, 10, 11,12,14)

= 0 RPP indicate the radial positions of pin rods.

= 1 RPP also play the role of RX. i.e. positions of annular division.

= 2 RPP further divide the pin rod regions into inner and outer regions.

Control of sub-division by RX, TY(effective for IGT=13, and 16)

= 0 with NTPIN $\neq$ 0, RXs and TYs do not divide coolant region, then only one coolant region is allocated to the region except pin rod regions

= 1 Division by RXs and TYs is effective. Usually enter IDIVP=1.

17 IBETM Range of angular integration in degree. (Effective for IGT=4 through 16)

Enter =45 in octant symmetric square geometry, =30 in hexagonal symmetry, Set double value if IBOUND=1 is specified. Enter =360 if symmetric only on left and right planes. Inefficient for one-dimensional geometry.

18 IPLOT Indicator to call plotter routine for geometry display

Plot data is stored as a PostScript file (cf. Sect.1.11)

= 0 Skip plotting

= 1 Call plotter routine (not effective for IGT=13,15,16)

Requirement of the following input Blocks are depending on geometries (IGT) specified in Block-1. It is summarized in Table 2.4-1.

Block-2 Iteration control parameters /7,6/

Parameters for the iterative solution of linear equations for neutron fluxes by the CPM. The value in < > shows defaulted value used when ITMINN ≤ 0 is specified. (cf. Sect.7.4)

1 IEDIT Edit control

= 0 No edit

plus 1 Print reaction balance and flux distribution

plus 2 Print macroscopic cross-sections

plus 4 Print collision probabilities

plus 8 Print fixed source distribution

Note:

If the user wants to print out macroscopic cross-sections and collision probabilities, IEDIT=2+4=6.

2 ITMINN Maximum number of inner iterations per an outer iteration

<20> for the eigenvalue problem, but <200> for the fixed source problem in thermal energy range

3 ITMOUT Maximum number of outer iterations for the eigenvalue problem <60>

4 ITBG Minimum number of iterations before extrapolation <5>

5 LCMX Number of iterations for testing over-relaxation factor <5>

6 ITDM Minimum delay between extrapolation <5>

7 IPT Control of monitor print at each iteration <0>

= 0 suppress print

= 1 print record

= -1 print detailed record

1 EPSI Convergence criterion for inner iterations <0.0001>

2 EPSO Convergence criterion for outer iterations <0.00001>

3 EPSG Extrapolation criterion <0.001>

4 RELC Initial over-relaxation factor <1.2>

5 OVERX Maximum extrapolation <100.>

6 FACTOR Under extrapolation factor <0.8>

Block-3 Required if NR<NZ /NZ/
NREG(*i*) T-Region number by Sub-Region (*i*)

Block-4 Required if NRR<NR /NR/
IRR(*i*) R-Region number by T-Region (*i*)

Block-5 Required if NXR<NRR /NRR/
IXR(*i*) X-Region number by R-Region (*i*).
If entered =0, this R-Region is excluded from the average in X-Region.

Block-6 /NRR/
MAR(*i*) Material number by R-Region (*i*)
Sequential order of a material appearing in the material specification in Sect.2.9 is used as material number.

=== Double heterogeneous problem option ===

Negative value of the material number indicates that this material is heterogeneous in the sense of the double heterogeneity[26]. For example, the coated particles dispersed in graphite matrix in the fuel compact of high temperature reactors compose the double heterogeneity. It is supposed that two composite materials of this material are specified in the preceding positions. That is, if the number -3 of an R-Region appears in MAR's, the first and second materials specified in Sect.2.9 are the composites of the microscopic cell. The relevant input data are required in Block-14. By this specification, both of microscopic and macroscopic heterogeneities are treated. The microscopic heterogeneity treated in this option is restricted to be two-region problem expressed by any of one-dimensional geometries (sphere, slab and cylinder) where the inner region is resonant and the outer is non-resonant. The double heterogeneous problem which

does not satisfy this condition must be treated in two-step process (cf. IXMICR in Sect. 2.9).

Block-7 Required only if IGT=10 or 14 and NAPIN $\neq 0$ /NAPIN/

NPIN(*i*) Number of pin rods on a circular ring (IGT=10) or on a hexagon (IGT=14).

If IGT=10, the pin rod on the central axis is not counted in NPIN. If IGT=14, the center pin rod is counted by NPIN. Defaulted values are prepared if NPIN(1)=0 is entered for IGT=14 as 1,6,12,18,....

Block-8 /NX+1/

RX(*i*) X-abscissa, radii, or the distances from the center to the flat of hexagon or square in unit of cm. Enter RX(1)=0 always.

Block-9 Required if IGT=11 or 12 and if NY>0 /NY/

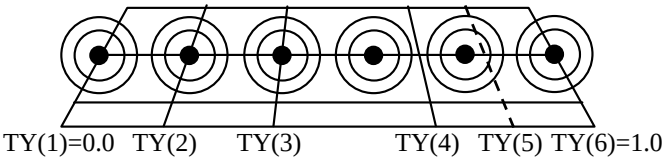
TY(*i*) Angular division by θ in degree

Block-9' Required if IGT=13 or 16 and if NY>1 /NY+1/

TY(*i*) Y-abscissa in cm. Enter TY(1)=0 always.

Block-9" Required if IGT=15 /NY+1/

TY(*i*) Division in anti-clockwise direction along the flat of outer trapezoidal regions by fraction. The region boundary line is drawn from the point expressed by the fraction to the center of hexagonal assembly. TY(1)=0.0 and TY(NY+1)=1.0 always. If the user wants to divide the flat into four equal pieces, enter 0.0, 0.25, 0.5, 0.75, 1.0. If a line crosses a pin rod, the line has to pass through the center of the pin rod. In the figure below, the line specified by TY(5) is not proper.



Block-10 Required if IGT=9,10 or 14 and NAPIN $\neq 0$ /NAPIN/

RPP(*i*) Positions (cm) of pin rods on X-direction for IGT=9.

Radii (cm) of the circles on which pin rods are located for IGT=10.

Distances (cm) from the center to the flats of hexagons for IGT=14.

Block-10’ Required if IGT=11, or 12 and NTPIN $\neq 0$ /NTPIN/

RPP(i) Radial position (cm) of each pin rod for IGT=11 or 12

Block-10” Required if IGT=13, 15, or 16 and NTPIN $\neq 0$ /NTPIN/

IXP(i) X-position of each pin rod on RX. Enter integers ranging from 1 to NX+1 for IGT=13, and =16, i.e. the lower left corner has the grid coordinate (1,1).

For IGT=15, the center of the assembly has the coordinate (0,0), then IXPs range from 0 to NX. While the input requires NTPIN entries, the entries for the first one-sixth part of a hexagon must be proper and others are dummy numbers because the 60° rotational symmetry is assumed.

Block-11 Required if IGT=10,11, or 12 and NTPIN $\neq 0$ /NTPIN/

THETA(i) Angular position of each pin rod by θ in degree

Block-11” Required if IGT=13, 15, or 16 and NTPIN $\neq 0$ /NTPIN/

IYP(i) Y-position of each pin rod on TY. Enter integers ranging from 1 to NY+1 for IGT=13 and 16, from 0 to NY for IGT=15. While the input requires NTPIN entries, the entries for the first one-sixth part of a hexagon must be proper and others are dummy numbers because the 60° rotational symmetry is assumed.

Block-12 Required if IGT=10 or 14 /NDPIN+1/

RDP(i) Radii (cm) for annular sub-division in a pin rod; where RDP(1)=0. The radii are common through all pin rods.

Block-12’ Required if IGT=9,11,12, 13, 15 or 16 and NTPIN $\neq 0$ /(NDPIN+1)*NTPIN/

RDP(i) Radii (cm) for annular sub-division of individual pin rod, where (RDP(1,j), j=1, NTPIN) =0 always.

For IGT=9, the input is required for an octant (1/8), then NTPIN= NAPIN*(NAPIN+1)/2.

For IGT=15, the entries for the first one-sixth part of a hexagon must be proper and others are dummy numbers because the 60° rotational symmetry is assumed.

Block-13 Plotter control integers, required if IPLOT $\neq 0$ in Block-1 is specified /3/

1 IG Signed integer to specify the combination of required region map; the integer is made of the summation of following integers corresponding to the kind of map.

= 0 None

plus 1 Sub-Region

plus 2 T-Region

plus 4 R-Region

plus 8 Material number

plus 16 X-Region

Note:

Positive value indicates printing of assignment of region numbers in the figure, and negative value requires only figure.

2 ISCAL Indicator of the scale of figures

= 1 One figure of diameter of 20 cm in a screen

= 2 Two figures of each diameter of 15 cm in a screen

= 3 Five figures of each diameter of 10 cm in a screen

3 ICONT Continuation indicator

= 0 Followed by the next Block-13

= 1 The last plotting

Block-14 Required if any negative MAR in Block-6 is entered /0,3,2/

Control integers for the treatment of the double heterogeneity

1 IDB Energy range indicator

= 1 Resonance range by the PEACO routine

= 2 Thermal range (not yet available)

= 3 Resonance and thermal range (not yet available)

2 IGEOM Geometry indicator of the microscopic heterogeneity

Restricted to two-region problem where the inner region is resonant and the outer is non-resonant.

= 1 Slab

= 2 Cylinder

= 3 Sphere

3 MODEL Model indicator for the definition of the collision rate ratio in the two-region microscopic cell.

= 1 Transmission (recommended)

= 2 Neutron from moderator

= 3 Neutron escaping from absorber lump

= 4 Simplified transmission

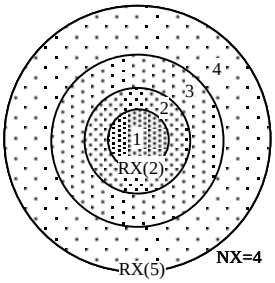
4 RF The thickness (cm) of absorber plate for IGEOM=1, and the outer radius (cm) of absorber lump for IGEOM=2,3.

5 RM The outer radius of microscopic cell. As the escape probability is evaluated by the analytical expression by Case *et al.*,[27] the Dancoff correction factor must be fed in the material specification in Sect.2.9 even if any is specified by IC3 in Sect.2.2.

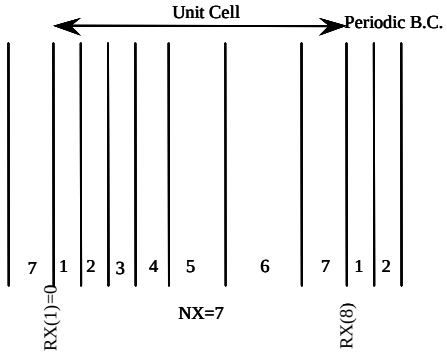
Table 2.4-1　List of input requirements for CPM routines by geometry model (IGT)

		IGT=1	IGT=2	IGT=3	IGT=4	IGT=5	IGT=6	IGT=7	IGT=8	IGT=9	IGT=10	IGT=11	IGT=12	IGT=13	IGT=14	IGT=15	IGT=16
B-1	IGT	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NZ	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NR	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NRR	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NRX	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	IBOUND	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NX	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NY	●	●	●	●	●	●	●	●	●	●	○	○	○	●	○	○
	NTPIN	●	●	●	●	●	●	●	●	●	○	○	○	○	○	○	○
	NAPIN	●	●	●	●	●	●	●	●	○	○	●	●	●	○	○	●
	NCELL	●	○	●	○	○	○	○	○	○	●	●	○	●	○	●	○
	IEDPIJ	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NGR	○	●	○	○	○	○	○	○	○	○	○	○	○	○	○	○
	NDA	●	●	●	○	○	○	○	○	○	○	○	○	○	○	○	○
	NDPIN	●	●	●	●	●	●	●	●	○	○	○	○	○	○	○	○
	IDIVP	●	●	●	●	●	●	●	●	○	○	○	○	○	○	●	○
	IBETM	●	●	●	○	○	○	○	○	○	○	○	○	○	○	○	○
	IPLOT	○	○	○	○	○	○	○	○	○	○	○	○	○	○	●	○
B-2	IEDIT～FACTOR	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
B-3	NREG	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△
B-4	IRR	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△
B-5	IXR	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△
B-6	MAR	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
B-7	NPIN	×	×	×	×	×	×	×	×	×	△	×	×	×	△	×	×
B-8	RX	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
B-9	TY	×	×	×	×	×	×	×	×	×	×	△	△	×	×	×	×
B-9'	TY	×	×	×	×	×	×	×	×	×	×	×	×	○	×	×	○
B-9''	TY	×	×	×	×	×	×	×	×	×	×	×	×	×	×	○	×
B-10	RPP	×	×	×	×	×	×	×	×	△	△	×	×	×	△	×	×
B-10'	RPP	×	×	×	×	×	×	×	×	×	×	△	△	×	×	×	×
B-10'	IXP	×	×	×	×	×	×	×	×	×	×	×	×	△	×	△	△
B-11	THETA	×	×	×	×	×	×	×	×	×	△	△	△	×	×	×	×
B-11'	IYP	×	×	×	×	×	×	×	×	×	×	×	×	△	×	△	△
B-12	RDP	×	×	×	×	×	×	×	×	×	△	×	×	×	△	×	×
B-12'	RDP	×	×	×	×	×	×	×	×	△	×	△	△	△	×	△	△
B-13	IG～ICONT	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△
B-14	IDB～RM	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△	△

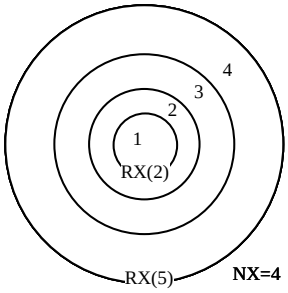
○: always required, ●: always required but ineffective, △: conditionally required, ×: not required



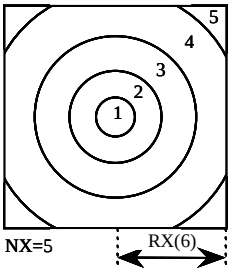
IGT=1 (Spherical cell)



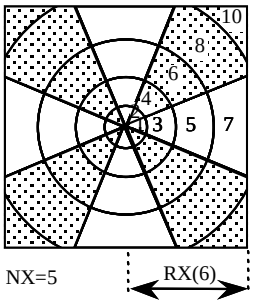
IGT=2 (Infinite plane cell)



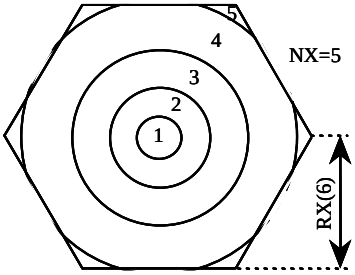
IGT=3 (Cylindrical cell)



IGT=4 (Square cell)

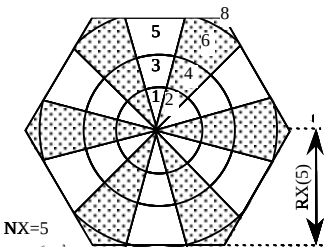


IGT=5 (2D square cell)

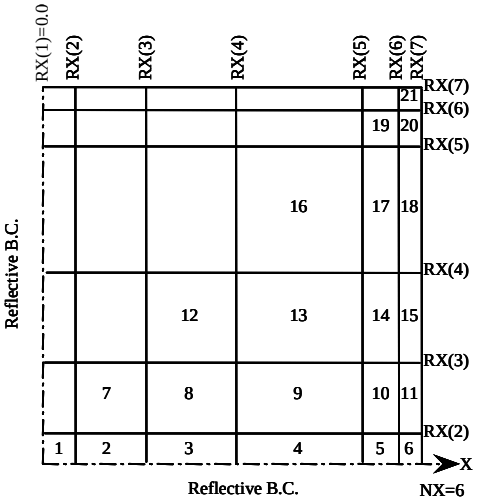


IGT=6 (Hexagonal cell)

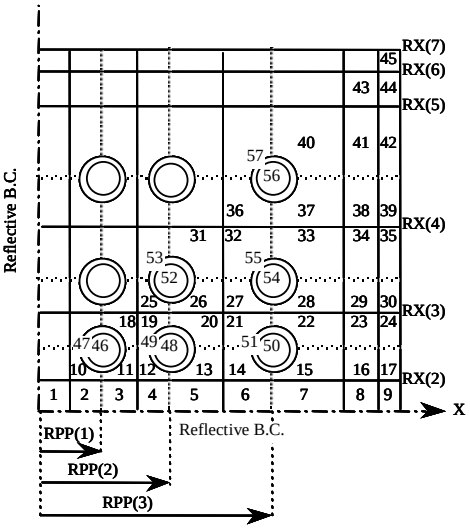
Fig.2.4-1 Geometries for PIJ (IGT=1~6)



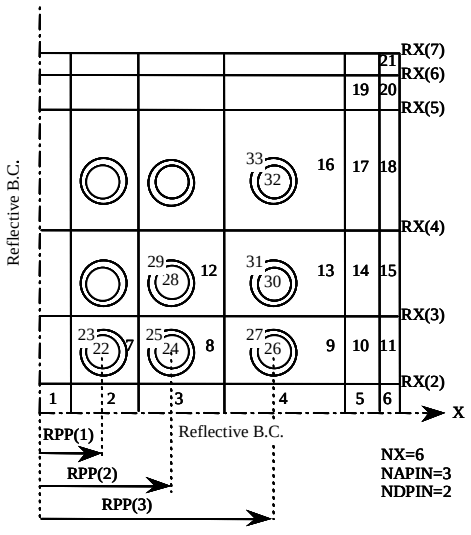
IGT=7 (2D hexagonal cell)



IGT=8 (Quadrant of an octant symmetric assembly)

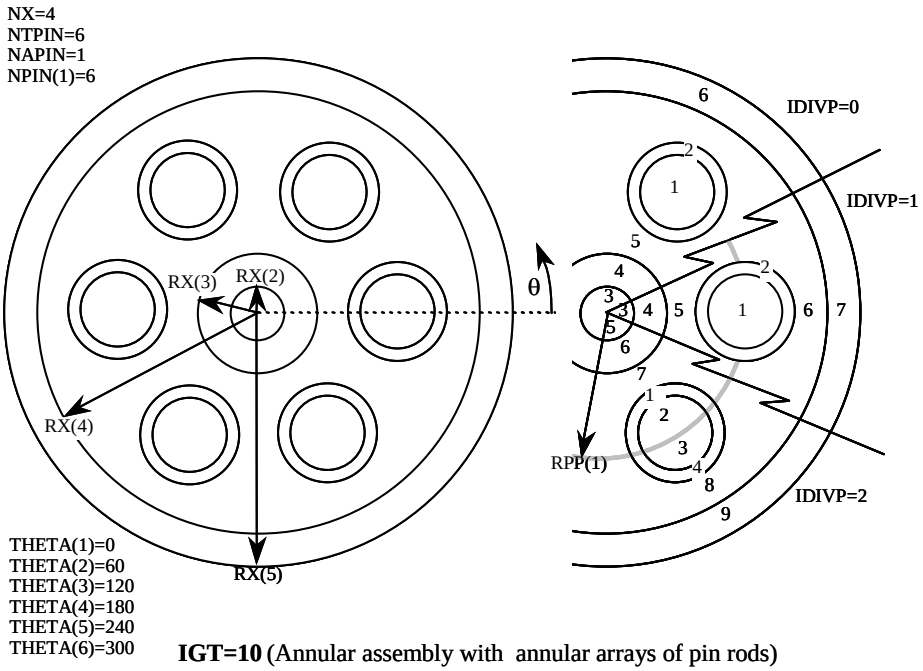


IGT=9 (Octant symmetric square assembly with pin rods)
IDIVP=1

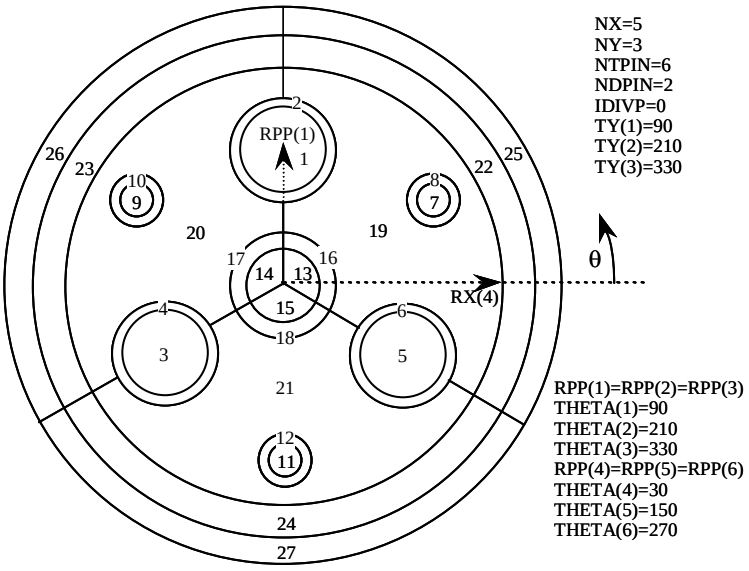


IGT=9 (Octant symmetric square assembly with pin rods)
IDIVP=0

Fig.2.4-2 Geometries for PIJ (IGT=7~9)

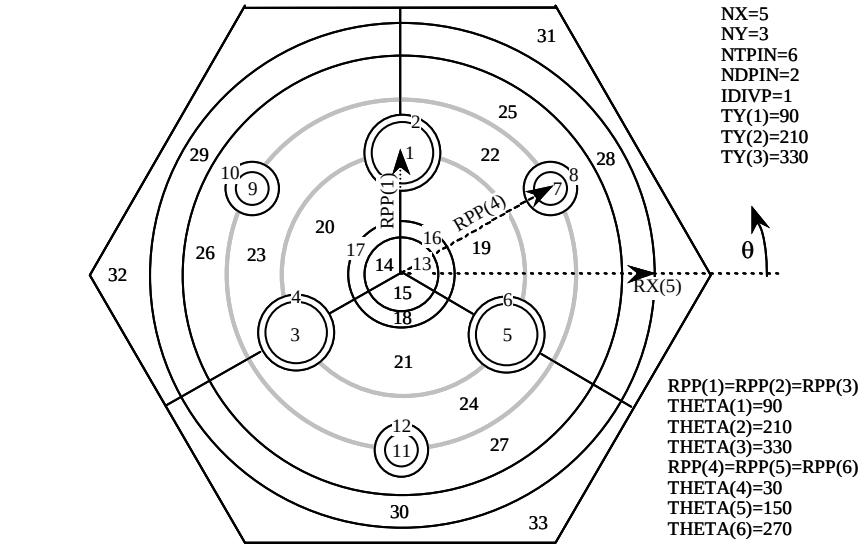


IGT=10 (Annular assembly with annular arrays of pin rods)



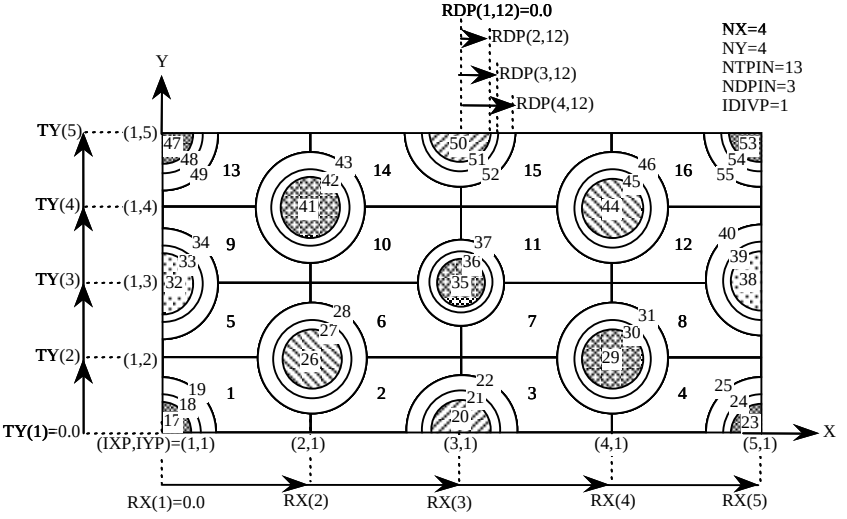
IGT=11 (Annular assembly with asymmetric pin rods)

Fig.2.4-3 Geometries for PIJ (IGT=10, 11)



If IDIVP=1, RPP(i) must not accross the pin rods on RPP(j) different from RPP(i).

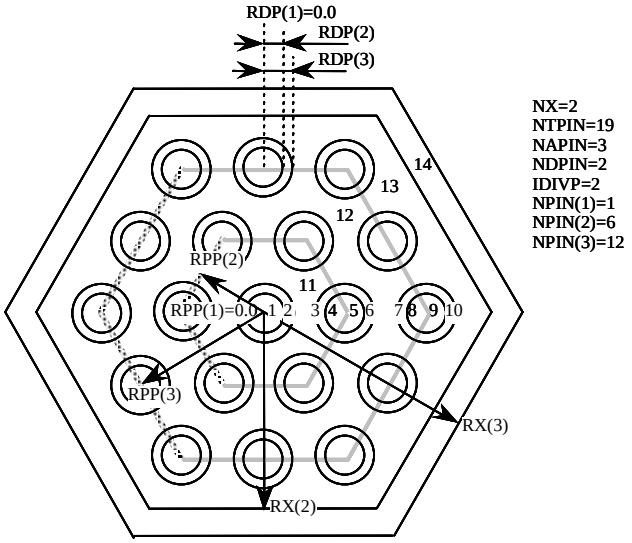
IGT=12 (Hexagonal assembly with asymmetric pin rods)



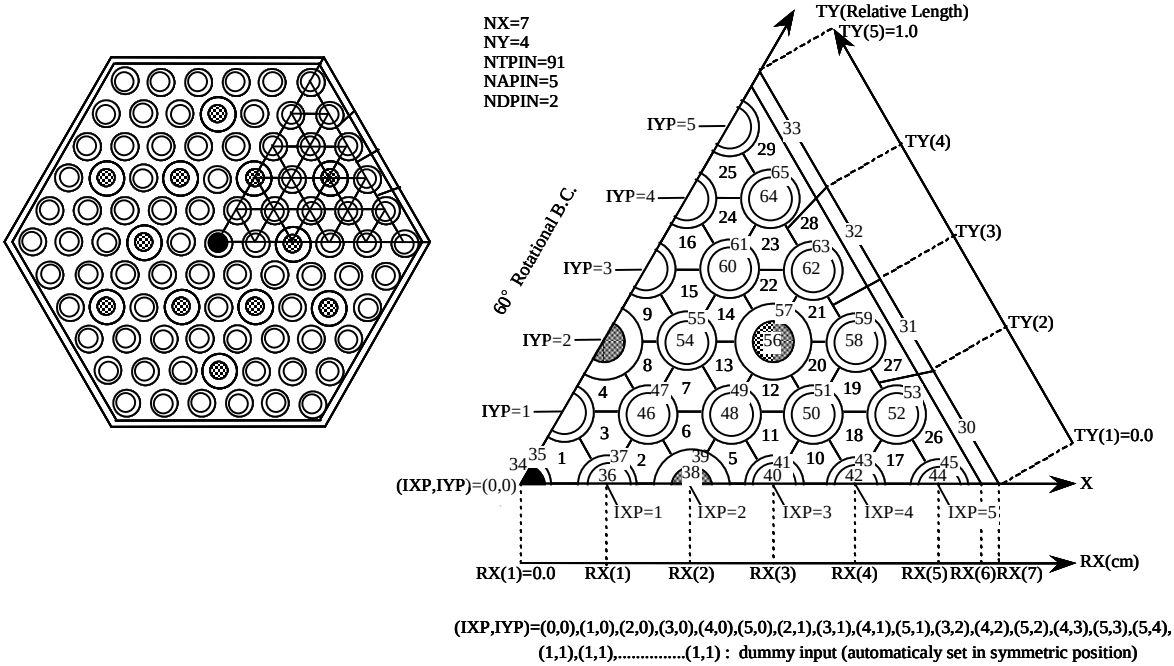
Sub-Region number for each pin rod is in order of (IXP,IYP).
(IXP,IYP)=(1,1), (3,1),(5,1),(2,2),(4,2),(1,3),(3,3),(5,3),(2,4),(4,4),(1,5),(3,5),(5,5)

IGT=13 (X-Y 2D cell with pin rods on arbitrary grid points)

Fig.2.4-4 Geometries for PIJ (IGT=12, 13)

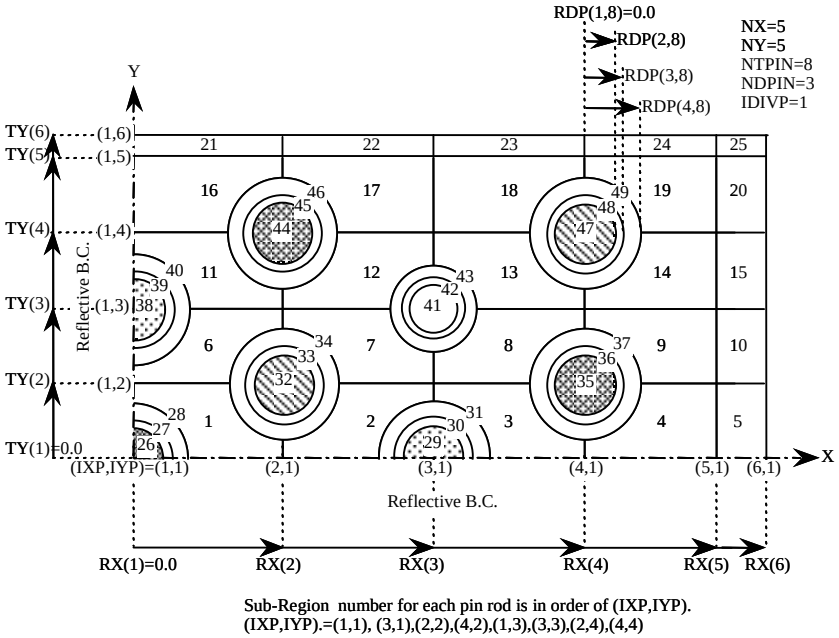


IGT=14 (Concentric layers of hexagons with equi-distant pin rod arrays)



IGT=15 (Hexagonal assembly with triangular pin rod arrangement)

Fig.2.4-5 Geometries for PIJ (IGT=14, 15)



IGT=16 (X-Y 2D symmetric cell with pin rods on arbitrary grid points)

Fig.2.4-6 Geometries for PIJ (IGT=16)

2.5 ANISN ; One-dimensional S_N Transport Calculation

The input of this section is required when the one-dimensional S_N routine ANISN is used by the specification IC2=2 or IC12=2/-2 (Sect.2.2) for either cell calculation or core calculation.

In the SRAC, the original ANISN[4)] is split into two steps. In the first step the reading the input and their check and storage into the arrays are executed. In the second step, the iterative procedure to obtain spectrum is executed. If IC2=2 is specified, the calculation is divided into the fast energy range and the thermal energy range with the fixed source fed by the SRAC. When IC12=2 is specified, the whole energy calculation with or without the external fixed source is executed. However, note that the external source is read in the second step. Therefore input data for the external source has to be given at the last of all input for a case.

Some functions permitted in the original ANISN are suppressed in the SRAC. As the macroscopic cross-sections are provided by the SRAC before executing the second step, the control integers relating to the cross-sections are internally set. As there is no essential change from the original ANISN, see the references[4)] of the ANISN for details.

The input format of the original ANISN (FIDO-format) is replaced by the the free format of SRAC described in Sect.2.1, however, the original key-codes specifying the array names and their orders are still kept to facilitate the reference to the original manual. The way of reading the arrays by indicating the array code of three characters is not changed except the replacement of '$' code by '&' code in the SRAC-ANISN.

< Example of input >

```
15&
1  0  4  2.............
16*
1.0  0.1  0.0001  1.420892...
.....................
00T
04*
.....................
27&
.....................
00T
```

& : input block for integer data

* : input block for floating point data

indicator for end of control data

indicator for end of ANISN input

Block-15& Integer parameters /36/

1 ID Problem ID number

Enter any number (not effective).

2 ITH Type of flux calculation to be performed

= 0 Forward solution

= 1 Adjoint solution

3 ISCT Maximum order of scatter found in any zone

= 0 P_0 component

= L P_L component (L=1~5)

The maximum order of scatter depends on the library selected (cf. Sect.8.2). Normally in the fine-group calculation, the scattering cross-sections up to P_5 are available for the material containing light water. (scattering matrices of order L>1 are prepared for limited light nuclides in the SRAC.)

In the few-group calculation, the P_1 calculation is available only when the P_1 cross-sections are prepared in the MACRO file as the result of collapsing of fine-group P_1 cross-sections after an anisotropic transport calculation by ANISN or TWOTRAN. Since the few-group cross-sections collapsed by the PIJ calculation do not include any higher order cross-sections, only P_0 (transport corrected) calculation is available.

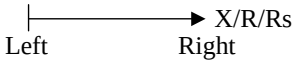
4 ISN Order of angular quadrature (S_N order)
Enter even integer (= 2/ 4/ 6/...../16..... ; S_2/ S_4/ S_6/..... /S_{16})

5 IGE Geometry

= 1 Slab (X)

= 2 Cylinder (R)

= 3 Sphere (R_S)



6 IBL Left boundary condition

= 0 Vacuum (no reflection)

= 1 Reflective

= 2 Periodic (angular flux leaving left boundary re-enters in the right boundary)

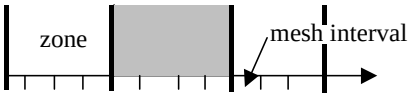
= 3 White / Albedo (some fraction returns isotropically)
The albedo values are entered in Block-26*.

7 IBR Right boundary condition, same as IBL

It is recommended that non-vacuum boundary at the right boundary for cylinder or sphere should be not reflective but white.

8 IZM Number of zones

A zone is composed by one or more spatial mesh. It is a unit for allocation of material, thus it is equivalent to an R-Region in the PIJ.



IZM=3, IM=11

9 IM Number of mesh intervals

10 IEVT Problem type

= 0 The fixed source mode calculation in SRAC (IC2=2 and IQM=1) or the external source problem in the whole energy range (IC12=±2 and IQM=2 or IPM>0). IQM and IPM is specified below in this Block

= 1 k_{eff} eigenvalue calculation

= 2 Time absorption α search

Note:

The search options on concentration (=3), zone width (=4), outer radius (=5) and buckling (=6) are all suppressed in the SRAC.

11 IGM Number of energy groups, required if Blocks 17*, 18*, 25*, 26* are read, otherwise enter 0 as it is internally set.

12 IHT Position of total cross-section in cross-section table

= 0 (internally set)

13 HIS Position of self-scatter cross-section in cross-section table

= 0 (internally set)

14 IHM Length of cross-section table

= 0 (internally set)

15 MS Cross-section mixing table length

= 0 (suppressed)

16 MCR Number of cross-section sets to be read from cards in the original format

= 0 (suppressed)

17 MTP Number of cross-section sets to be read from tape

= 0 (internally set)

18 MT Total number of cross-section sets

= 0 (internally set)

19 IDFM Control for density factors

= 0 (suppressed)

20 IPVT Indicator of the parametric eigenvalue PV entered in Block-16* for the search options (IEVT>1).

This term is effective when IEVT=2, because other search options are suppressed in the SRAC. Enter 0 when IEVT=0 or 1, otherwise(IEVT=2) enter =1.

= 0 PV is not effective: ANISN will search for the parameter to make k_{eff}=1.0 with α=0.0. (suppressed)

= 1 PV as k_0: ANISN will search for the parameter to make k_{eff}= k_0.
Usually, PV= k_0=1.0 for α search.

= 2 PV as α_0 : ANISN will search for the parameter to make k_{eff}=1.0 when α =α_0. (suppressed)

21 IQM Indicator of distributed source

= 0 No distributed source in eigenvalue problem.

= 1 Distributed source formed in the SRAC.
The energy spectrum of U-235 fission spectrum with spatially flat source on the zone which has non-zero fission cross-sections are given.

= 2 Isotropic distributed source read from Block-17* in execution step of ANISN.

22 IPM Angular dependent incident source on the right surface of the mesh interval (shell source)

= 0 No shell source.

= 1 Shell source on one mesh.
The position of the mesh is specified by the next input (IPP).
Enter shell source by group and angle in Block-18*.

= IM Shell source on every mesh points.
IM is the number of mesh intervals specified in the 9-th input of this Block. Enter shell source by interval, group, and angle in Block-18*.

23 IPP Position of the mesh interval on which shell source is given by IPM=1.

= 0 if IPM $\neq$ 1

= N interval number which contains the shell source if IPM=1

24 IIM Inner iteration maximum (suggested value, IIM = 35)

25 ID1 Printing of angular flux

= 0 No effect

= 1 Print angular flux

26 ID2 Special cross section tape

= 0 (suppressed)

27 ID3 Reaction rate calculation by zone

= 0 No effect

= N Compute N activities by zone. See Block-22& and -23&

28 ID4 Reaction rate calculation by mesh interval

= 0 No effect

= 1 Compute N (specified by ID3) activities by interval

29 ICM Outer iteration maximum
A suggested value is 50.

30 IDAT1 Auxiliary tape storage of data

= 0 (suppressed)

31 IDAT2 Diffusion theory solution for partial groups

= 0 (suppressed)

32 IFG Weighted cross-sections

= 0 (suppressed)

33 IFLU Control for extrapolation model

= 0 Use mixed model: step model is used when linear extrapolation yields negative flux (suggested option)

= 1 Use linear model only

= 2 Use step model only

34 IFN Control for initial guess

= 0

Note: In SRAC, IFN is internally set depending on problems; IFN=0 for eigenvalue problem, and IFN=1 for fixed source problem.

Originally, INF=0: Enter fission guess, =1: Enter flux guess, =2: Use fluxes from previous case

35 IPRT Control for printing of cross-sections

= 0 Print cross-sections

= 1 Skip printing

36 IXTR P_L constants to be used

= 0 Calculate P_L scattering constants as Legendre coefficients, (suggested option)

= 1 Read P_L constants entered in Block-34*

Block-16* Floating point parameters /14/

1 EV Initial guess for eigenvalue

EV = 0.0 when IEVT=0 or 1

EV = best guess for α or 0.0 when IEVT=2

2 EVM Eigenvalue modifier for the first eigenvalue change

$EV^1 = EV^0 + EVM$, after the first modification, the linear or the quadratic extrapolation is internally executed.

3 EPS Convergence criterion (accuracy desired)

(suggested value: EPS=0.0001)

4 BF Buckling factor

Normally enter 1.420892, if so the extrapolation length of group *g*:

$$\delta_g = 0.710446 * \lambda_{tr,g}$$

ANISN computes a correction factor of the $D_g B^2$ form for the finite transverse dimensions. In the evaluation of B^2, $2\delta_g$ is added to the transverse dimensions.

$$D_g B^2 = \frac{1}{3\Sigma_{t,g}} \left\{ \frac{\pi^2}{\left(DY + 2\delta_g\right)^2} + \frac{\pi^2}{\left(DZ + 2\delta_g\right)^2} \right\},$$

$$2\delta_g \equiv BF * \lambda_{t,g} = BF / \Sigma_{t,g}$$

To evaluate B^2 without the extrapolation length $2\delta_g$, enter BF=0.0.

$\Sigma_{t,g}$ is a total cross-section if it is prepared by anisotropic calculation routine ANISN or TWOTRAN, otherwise $\Sigma_{t,g}$ is a transport cross-section, because these cross-sections are stored in the same position in MACRO file.

5 DY Cylinder or plane height (cm) for buckling correction

DY may include extrapolation length when BF=0.0.

6 DZ Plane depth (cm) for buckling correction

DZ may include extrapolation length when BF=0.0.

7 DFM1 Transverse dimension for void streaming correction (Usually DFM1=0.0)

When a void region is included in the system, the evaluation of transverse leakage by the buckling approximation is not suitable. A simple correction[28)] is provided by removing the angular component of transverse direction in the void region. As this correction does not introduce the pseudo absorption due to

transverse leakage, the neutron balance in the system is not satisfied. This correction does not work if DFM1=0.0 is entered.

8 XNF Normalization factor for fission source

If XNF=0.0, no normalization is done. (suggested option)

If XNF $\neq$ 0.0 and IEVT>0, the total fission source is normalized to XNF.

If XNF $\neq$ 0.0 and IEVT=0, The total fixed source is normalized to XNF and the fission source, if any, is not normalized.

9 PV Parametric eigenvalue (k_0 or α_0) to be converged in the search calculation (effective for IEVT>1)

If IPVT=0, PV=0.0,

If IPVT=1, PV= k_0 (Usually, k_0=1.0 for α search)

If IPVT=2, PV= α_0

10 RYF Relaxation factor for the convergence criterion of total scattering and up-scattering.

The criterion =EPS/RYF (suggested value = 0.5)

11 XLAL Point flux convergence criterion in the inner iterations if XLAL>0.0.

(suggested value = 2.0*EPS)

12 XLAH Search control parameter (effective if IEVT>1)

Upper limit for $\left|1.0-\lambda_1\right|$ used in the linear search.

Normally, XLAH = 0.05.

13 EQL Search control parameter (effective if IEVT>1)

When $\left|\lambda_1^{New}-\lambda_1^{Old}\right|$<EQL is satisfied, the eigenvalue is changed.

Normally, 0.001< EQL < 3*EPS.

14 XNPM Search control parameter (effective if IEVT>1)

New parameter modifier to prevent oscillation in the linear search calculation.

Normally, XNPM=0.75.

Block-00T Termination of control numbers /A3/

Enter ’00T’.

Block-04* Positions of interval boundary /IM+1/

Enter the distances from the origin in cm including the origin (0.0).

Block-06* Angular quadrature weights /MM/

MM = ISN + 1 for plane or sphere

MM = ISN*(ISN+4)/4 for cylinder

For ISN= 2, 4, 6, 8, 12, and 16, built-in constants are prepared, then no entry is required.

Block-07* Angular quadrature cosines /MM/

For ISN = 2, 4, 6, 8, 12, and 16, built-in constants are prepared; then no entry required.

Block-08& Zone number by mesh interval /IM/

Block-09& Material number by zone /IZM/

Material number is allocated by the position of the material name appearing in the material specifications (Sect.2.9).

The function activated by the negative value to suppress the buckling effect is removed in the SRAC.

Block-19& Order of scatter (P_L) by zone /IZM/

Block-22& Material numbers for activity calculation, required if ID3>0 in Block-15& /ID3/

Block-23& Cross-section table position for activities, required if ID3>0 /ID3/

Block-25* Albedo by group for right boundary, /IGM/

required if IBR=3 in Block-15& (7) and albedo is used

Block-26* Albedo by group for left boundary, /IGM/

required if IBL=3 in Block-15& (6) and albedo is used

Block-27& X-Region number /IZM/

X-Region number by zone to indicate the region where the cross-sections are averaged by flux*volume weight

Block-34* P_L scatter constants by angular point, /JT*MM/

required if IXTR=1 in Block-15& (36)

JT=ISCT	for plane or sphere
JT = ISCT*(ISCT+4)/4	for cylinder

See Block-06* for MM.

Block-00T Termination card to indicate the end of ANISN input /A3/
Enter '00T'.

The following Blocks are required if the external source problem is solved by specifying IQM=2 or IPM=1. As the external source input is read in the execution step of ANISN, it must be positioned after PEACO input (Sect.2.12).

Block-17* Distributed source, if IQM=2 in Block-15& (21) /IM*IGM/
($Q_d(i,g)$, i=1,IM), g=1,IGM); Enter Q_d in the order as
$Q_d(1,1)$, $Q_d(2,1)$,…., $Q_d(IM,1)$, $Q_d(1,2)$,….., $Q_d(IM,2)$, …, $Q_d(IM,IGM)$
IM: number of mesh intervals in Block-15& (9), IGM: number of groups in Block-15& (11)

Block-18* Shell source, if IPM=1 in Block-15& (22) /MM*IPM*IGM/
Angular dependent incident source at angular point m, spatial mesh point i, group g
if IPM=1, (($Q_s(m,g)$, m=1,MM), g=1,IGM)
if IPM=IM, ((($Q_s(m,i,g)$, m=1,MM), i=1,IM), g=1,IGM)
See Block-06* for MM.

2.6 TWOTRAN ; Two-dimensional S_N Transport Calculation

This section describes the input requirements of the two-dimensional S_N routine TWOTRAN required when IC2=3 or IC12=3 is specified in Sect.2.2. This code can be used either in cell calculation or core calculation. In the SRAC, the original TWOTRAN[5] is split into two steps. In the first step reading the input and their check and storage into the arrays are executed. In the second step, the iterative procedure to obtain spectrum is executed. If IC2=3 is specified, the calculation is divided into the fast energy range and the thermal energy range with the fixed source fed by the SRAC. When IC12=3 is specified, the whole energy calculation with or without the external fixed source is executed. However, note that the external source is read in the second step. Therefore input data for the external source have to be given at the last of all input for a case.

Some functions permitted in the original TWOTRAN are suppressed in the SRAC. As the macroscopic cross-sections are provided by the SRAC before executing the second step, the control integers relating to the cross-sections are internally set. As there is no essential change from the original TWOTRAN, see the references[5] of the TWOTRAN for details.

The input format of the original TWOTRAN is replaced by the free format of SRAC described in Sect.2.1, however, the original array names and their orders are still kept to facilitate the reference to the original manual.

Block-1 /1/

NTITLE Number of comment cards

Block-2 (NTITLE)*/A72/

TITLE Job title or job description.

Block-3 Control integers /42/

1 ITH Type of flux calculation to be performed

= 0 Forward solution

= 1 Adjoint solution

2 ISCT Order of scattering calculation.

There are NM=(ISCT+1)(ISCT+2)/2 spherical harmonic scattering source components computed. There are not used to compute a scattering source unless

any of zone material identification numbers is negative. See IDCS in Block-16.

= 0 Isotropic scattering

= 1 P_1 scattering

= L P_L component (L=1~5)

Note:

The maximum order of scatter depends on the library selected (cf. Sect.8.2). Normally in the fine-group calculation, the scattering cross-sections up to P_5 are available for the material containing light water. (scattering matrices of order L>1 are prepared for limited light nuclides in the SRAC.)

In the few-group calculation, the P_1 calculation is available only when the P_1 cross-sections are prepared in the MACRO file as the result of collapsing of fine-group P_1 cross-sections after an anisotropic transport calculation by ANISN or TWOTRAN. Since the few-group cross-sections collapsed by the PIJ calculation do not include any higher order cross-sections, only P_0 (transport corrected) calculation is available.

3 ISN Order of angular quadrature (S_N order)

Enter even integer (= 2/ 4/ 6/...../16..... ; S_2/ S_4/ S_6/..... /S_{16})

If negative, quadrature coefficients are taken from the 11th logical device. Otherwise (for ISN from 2 through 16) built-in constants are used.

4 IGM Number of energy groups (internally set)

5 IM Number of rebalance coarse mesh intervals in the *i*-direction.

IM=3 in the example of Fig.2.6-1.

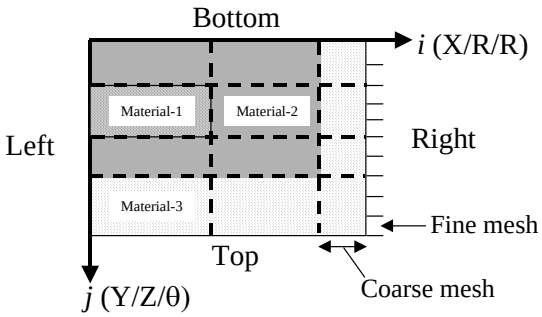


Fig.2.6-1 Cordinates in TWOTRAN

Note:

The original TWOTRAN uses two coarse mesh concepts: rebalance coarse mesh and material coarse mesh. In the SRAC code, both of these coarse mesh divisions are treated as the same zone division to be used for material allocation. See entries IMC (40th term in this Block).

6 JM Number of rebalance coarse mesh in the *j*-direction.
JM=4 in the example of Fig.2.6-1.
See entries JMC (41st term in this Block).

7 IBL Left boundary condition (See Fig.2.6-1)
= 0 Vacuum
= 1 Reflective

8 IBR Right boundary condition
= 0 Vacuum
= 1 Reflective
= 2 White

9 IBB Bottom boundary condition
= 0 Vacuum
= 1 Reflective
= 2 White
= 3 Periodic

Note:

The definition of ’Bottom’ and ‘Top’ is reversed to that of CITATION.

10 IBT Top boundary condition
= 0 Vacuum
= 1 Reflective
= 2 White
= 3 Periodic (if IBB=3)

11 IEVT Eigenvalue type

= 0 The fixed source mode calculation in SRAC (IC2=3 and IQOPT=0) or the external source problem with inhomogeneous source option in the whole energy range (IC12=3 and IQOPT>0). IQOPT is specified below in this Block.

= 1 k_{eff} calculation

= 2 Time absorption α search

= 3 Nuclide concentration search (suppressed)

= 4 Zone thickness (delta) search (suppressed)

12 ISTART Input flux guess and starting option

= -5 Entire scalar flux guess from logical device 33

= 0 No flux guess required, but a fission guess (uniform in fissionable zone) is automatically supplied

= 6 Problem restart dump is read from logical device 12

Other options in this item are suppressed.

13 MT Total number of cross-section blocks including anisotropic cross-sections. If ISCT=0, this item is equal to number of materials used.

14 MTPS Number of input material set from the interface file ISOTXS supplied by SRAC. As the next item MCR is set to zero, this item is identically equal to the number of materials.

15 MCR Number of input materials from the code dependent input file,

= 0 (suppressed)

16 MS Number of mixture instructions

= 0 (suppressed)

17 IHT Row position of total cross-section in the cross-section format

= 0 (internally set)

18 HIS Row position of within-group scattering cross-section in the cross-section format

= 0 (internally set)

19 IHM Total number of rows in the cross-section format

= 0 (internally set)

20 IQOPT Option for input inhomogeneous source;

Qgijn, for *g*=1,IGM, *i*=1,IT, *j*=1,JT, *n*=1,NMQ

where NMQ = (IQAN+1)(IQAN+2)/2, and IQAN is given by next item.

IT/JT is total number of fine mesh in *i*/*j*-direction, equal to the sum of IHX/IHY vector in Block-5/6.

= 0 No input required; fixed source mode calculation (IC3=3,IEVT=0) or eigenvalue problems (IC12=3,IEVT>0).

When the fixed source mode calculation is specified, in fast neutron energy range a fission neutron spectrum of spatially flat and isotropic source will be supplied automatically. For the thermal neutron range spatially flat slowing-down source in each zone will be supplied automatically.

= 1 Enter the energy spectrum $GR(g,n)$ for each angular component *n* in Block-7, where spatially flat source is assumed.

$Qgijn = GR(g,n)$

= 2 Enter an energy spectrum and NMQ sets of spatial shape (in Block-7)

$Qgijn = G(\mathrm{g})*R_n(i,j)$, n=1,NMQ

$Q(i,j,n,g) = (((Q(i,j,n,g), i=1,\mathrm{IT}), j=1,\mathrm{JT}), n=1,\mathrm{NMQ}), g=1,\mathrm{IGM})$

= 3 Enter first a spectrum and a shape IT*JT, then repeat for *n.* (in Block-7)

$Qgijn = G_n(\mathrm{g})*R_n(i,j)$, n=1,NMQ

= 4 Enter first a spectrum and an *i*-direction shape, and a *j*-direction shape, then repeat for *n*. (in Block-7)

$Qgijn = G_n(\mathrm{g})*X_n(i)*Y_n(j)$, n=1,NMQ

= 5 The complete source is read from interface file (FIXSRC) on logical device 32.

21 IQAN Order of anisotropy of inhomogeneous distributed source

= 0 Isotropic

= L L-th order of anisotropy

22 IQR Right boundary source to be specified as input.

= 0 No source

= 1 Read source by Block-8, -9

23 IQB Bottom boundary source to be specified as input.

= 0 No source

= 1 Read source by Block-10, -11

24 IQT Top boundary source to be specified as input.

= 0 No source

= 1 Read source by Block-12, -13

25 IPVT Indicator of the parametric eigenvalue PV entered in Block-4 for the search options (IEVT>1). This term is effective when IEVT=2, because other search options are suppressed in the SRAC. Enter 0 when IEVT=0 or 1, otherwise(IEVT=2) enter =1.

= 0 PV is not effective: TWOTRAN will search for the parameter to make k_{eff}=1.0 with α=0.0. (suppressed)

= 1 PV as k_0: TWOTRAN will search for the parameter to make k_{eff}= k_0. Usually, PV= k_0=1.0 for α search.

= 2 PV as α_0 : TWOTRAN will search for the parameter to make k_{eff}=1.0 when $\alpha=\alpha_0$. (suppressed)

26 IITL Maximum number of inner iterations allowed per group

27 IXM *i*-direction zone thickness modifier (suppressed)

28 IYM *j*-direction zone thickness modifier (suppressed)

29 ITLIM Time limit in CPU, if an integer of seconds is entered, a restart dump is taken after this number of seconds and the job is terminated.

30 IGEOM Geometry

= 1 X-Y

= 2 R-Z

= 3 R-θ

31 IEDOPT Edit options.

= 0 None

= 1 Macroscopic edit

= 2 (suppressed)

= 3 Option 1 plus a zone relative power density edit

= 4 (suppressed)

32 ISDF Indicator to density factor input

= 0 No

= 1 Yes (suppressed)

33 I1 Full input flux print suppression indicator

= 0 Print

= 1 No print

34 I2 Final flux print indicator

= 0 All

= 1 Isotropic

= 2 None

35 I3 Cross-section print indicator

= 0 All

= 1 Mixed (suppressed)

= 2 None

36 I4 Final fission distribution print indicator

= 0 Yes

= 1 No

37 I5 Source input print indicator

= 0 All

= 1 Input values only

= 2 Normalized values

= 3 None

38 I6 Indicator to prepare and print coarse-mesh balance tables

= 0 Yes

= 1 No

Note:

The tables are for the rebalance mesh when the rebalance mesh and material mesh are different. (always same in the SRAC)

The preparation of these tables requires an additional outer iteration after problem convergence.

39 IANG Edit for angular fluxes. The preparation of angular fluxes requires an additional outer iteration after problem convergence as well as additional storage.

= -1 Print and store on logical device 8

= 0 None

= 1 Store on logical device 8

40 IMC Number of material coarse-mesh intervals in the *i*-direction.

= 0 (suppressed)

Note:

When this value is non-zero, the rebalance coarse-mesh as given by items IM and JM is not the same as the material coarse-mesh. The material coarse-mesh is the same as the mesh upon which all edits are done. When edits are requested and IMC is not zero, angular fluxes must be stored. See entries IDCS, XM, IHXC, and XRAD below.

41 JMC Number of material coarse-mesh intervals in the *j*-direction.

= 0 (suppressed)

42 IF0 Interface file output is created. Total (angle-integrated) flux on ITFLUX (=33) and angular weight constants on ISNCONS(=11) files are always created. Angular flux file is created on LAFLUX (=9) only if IANG is not zero.

= 0 No

= 1 Yes

Block-4 Control floating point data /10/

1 EV Eigenvalue guess. It is satisfactory to enter EV=0.0 in SRAC.

2 EVM Eigenvalue modifier used only if IEVT>1.
$EV^1=EV^0+EVM$

3 PV Parametric eigenvalue (k_0 or α_0) to be converged in the search calculation (effective for IEVT>1)
If IPVT=0, PV=0.0,
If IPVT=1, PV= k_0 (Usually, k_0=1.0 for α search)
If IPVT=2, PV= α_0

4 XLAL Lambda lower limit for eigenvalue searches (effective if IEVT>1)
lambda is the ratio of (Fission source + Inhomogeneous source, if any) in two succeeding iterations.

5 XLAH Search lambda upper limit (effective if IEVT>1).

6 XLAX Search lambda convergence precision for second and subsequent values of the eigenvalue (effective if IEVT>1).

7 EPS Convergence precision.

8 NORM Normalization factor. Total number of particles in system is normalized to this number if NORM>0. No normalization if NORM=0.

9 POD Parameter oscillation dumper used in eigenvalue searches (effective if IEVT>1).
$POD \leq 0.5$ is recommended for α search.

10 BHGT Sighed value of buckling height in cm used to simulate the axial leakage by adding a pseudo absorption given by

$$\Sigma_{a,g}^{eff} = \Sigma_{a,g} + D_g B^2 \quad , \quad 2\delta_g = 2 * 0.710446 \lambda_{tr,g} = 1.420892 / \Sigma_{t,g}$$

$$D_g B^2 = \frac{1}{3\Sigma_{t,g}} \left\{ \frac{\pi^2}{\left(BHGT + 2\delta_g\right)^2} \right\} = \frac{\Sigma_{t,g}}{3} \left\{ \frac{\pi^2}{\left(\Sigma_{t,g} * BHGT + 1.4209\right)^2} \right\}$$

Here $2\delta_g = 1.4209 / \Sigma_{t,g}$ is twice the Milne problem extrapolation distance. $\Sigma_{t,g}$ is a total cross-section if it is prepared by anisotropic calculation routine ANISN or TWOTRAN, otherwise $\Sigma_{t,g}$ is a transport cross-section, because these cross-sections are stored in the same position in MACRO file.

Use this option in (X,Y) and (R,θ) geometries only. If the negative value is entered, the Milne extrapolation distance is not added to the buckling height.

Block-5 /IM/

IHX(*i*) Number of fine mesh intervals in each coarse-mesh *i*-interval.

Block-6 /JM/

IHY(*j*) Number of fine mesh intervals in each coarse-mesh *j*-interval.

Block-14 /IM+1/

XRAD(*i*) Coarse *i*-mesh boundaries in cm. Must form increasing sequence including the original point (0.0).

Block-15 /JM+1/

YRAD(*j*) Coarse *j*-mesh boundaries in cm. Must form increasing sequence including the original point (0.0).

Block-16 /IM*JM/

IDCS(*i*,*j*) Material identification numbers by coarse mesh zone.

Material number is assigned by the order appearing in the material specifications in Sect.2.9. Enter in the order : (IDCS(*i*,*j*),*i*=1,IM),*j*=1,JM).

If these numbers are negative, an anisotropic scattering source is calculated in the coarse mesh zone; but the numbers need not be negative unless ISCT>0.

----- A sample input for Fig.2.6-1 -----

```
-2 -2 -3 / j=1
-1 -2 -3 / j=2
-2 -2 -3 / j=3
-3 -3 -3 / j=4=JM
```

（Note : This map will be printed inversely)

Block-19 Required if IEDOPT>0 (See 31st term in Block-3) /1/

NEDS Number of edits to be performed (See below)

Repeat Block-20 through Block-21, NEDS times.

Block-20	Required if NEDS>0	/2/
NZ	Integer of edit zones.	
NORMZ	The zone to which the power density is normalized. (effective if IEDOPT=3 or =4) Normalized to average value of the whole system if NORMZ=0.	
Block-21	Required if IEDOPT>0	/IM*JM/
NEDZ(*i*,*j*)	Integers defining which edit zone each coarse mesh material zone is in.	
Block-22		/IM*JM/
IXZ(*i*,*j*)	X-Region numbers by coarse mesh zone.	

The following distributed and boundary sources Blocks -7, -8, -9, -10, -11, -12, and -13 are read in the execution step of TWOTRAN; they must be positioned after the PEACO input data.

Block-7	Required if IQOPT=1,2,3,4 (See 20th term in Block-3)	/See option IQOPT/
Q(*g*,*i*,*j*,*n*)	External volume source depending on IQOPT	
	if IQOPT =1 NQM set of IGM	
	if IQOPT=2 IGM groups of NMQ blocks of IT*JT	
	if IQOPT=3 NMQ sets of IGM and IT*JT	
	if IQOPT=4 NMQ sets of IGM and IT then JT	
	if IQOPT=5 entire source from logical device 32	
	where IT= $\sum_{i=1}^{IM}$ IHX(*i*), JT= $\sum_{j=1}^{JM}$ IHY(*j*)	
Block-8	Required if IQR=1 (See 22nd term in Block-3)	/JT*MM/
QR1(*j*,*n*)	Right boundary source (flux) in the in-down directions. JT is total number of fine mesh in *j*-direction, equal to the sum of IHY vector in Block-6, and MM is total number of angular mesh in a quadrant; MM= ISN*(ISN+2)/8.	
Block-9	Required if IQR=1	/JT*MM/
QR2(*j*,*n*)	Right boundary source (flux) in the in-up directions.	
Block-10	Required if IQB=1	/IT*MM/

QB1(*i*,*n*)	Bottom boundary source (flux) in the in-up directions. IT is total number of fine mesh in i-direction, equal to the sum of IHX vector.	
Block-11	Required if IQB=1	/IT*MM/
QB2(*i*,*n*)	Bottom boundary source (flux) in the out-up directions.	
Block-12	Required if IQT=1	/IT*MM/
QT1(*i*,*n*)	Top boundary source (flux) in the in-down directions.	
Block-13	Required if IQT=1	/IT*MM/
QT2(*i*,*n*)	Top boundary source (flux) in the out-down directions.	

2.7 TUD ; One-dimensional Diffusion Calculation

The one-dimensional diffusion routine TUD is preferred to the CITATION by the simpler input requirement. The following data are required if IC2=4 or IC12=4 is entered in Sect.2.2.

Block-1 Control integers /9/

1 NRMAX Number of regions

A region is divided into fine mesh intervals for flux calculation by the finite difference method. Material (a set of cross-sections) is assigned by region.

2 IG Geometry type

= 0 Slab (X)

= 1 Cylinder (R)

= 2 Sphere (R_S)

3 IBOUND Outer boundary condition

= -1 Zero flux at the outer boundary

= 0 Reflective

= 1 Zero flux at the group dependent extrapolated distance calculated by using the Milne problem constant: 0.71045.

= 2 Zero flux at the extrapolated distance by using the constant entered by Block-9

Note: The boundary condition at $\vec{r} = 0$ is always set as reflective.

4 IGUESS Initial flux guess control

= -1 Read from logical device 33 prepared by the user

= 0 Uniform; no input required

= N Read from logical device 10 in binary mode as written by ITFLUX below

5 IPTXEC Print control for cross-sections

= 0 Skip print

= 1 Print

6 ITFLUX Print control for fine flux distribution

= 0 Skip print

= 1 Print

= 4 Write on logical device 33 by the statement

WRITE(33) ((F(*i*, *g*), *i*=1,NNMAX+1), *g*=1,NGMAX)

where F(*i*,*g*) = $\varphi_g(r_i)\Delta E_g$ for Slab, Cylinder

= $r_i\varphi_g(r_i)\Delta E_g$ ($r \neq 0$) and $\varphi(0)\Delta E_g$ (r=0) for Sphere

= 5 Action 1 and 4

7 IPS Print control for the fixed source distribution.

= 0 Skip print

= 1 Print

8 IDOPT Selection of the diffusion coefficients (cf. IC17 in Sect.2.2)

= 1 use D1 in the macroscopic cross-section organization

= 2 use D2 in the macroscopic cross-section organization

9 NXR Number of X-Regions

Block-2 Integer parameters for the iterative process /6/

If entered =0 for each following integer, the value in < > is substituted.

1 ITMIN Maximum number of inner iterations in thermal neutron energy range per outer iteration.

< 100 > for the fixed source problem

< 10 > for the eigenvalue problem

2 ITMOUT Maximum number of outer iterations < 25 >

3 ITBG Minimum number of inner iterations before extrapolation < 5 >

4 LCMX Number of inner iterations for testing over-relaxation factor < 5 >

5 ITDM Minimum delay between extrapolation < 5 >

6 IPT Control for monitor print < 0 >

= 0 Skip print

= 1 Monitor print at each inner iteration

Block-3 Floating point parameters /6/
If entered =0.0 for each following item, the value in < > is substituted.

1 EPSI Convergence criterion for inner iteration < 0.001 >

2 EPSO Convergence criterion for outer iteration < 0.0001 >

3 EPSG Extrapolation criterion < 0.001>

4 RELC Initial over-relaxation factor < 1.2 >

5 OVERX Maximum extrapolation factor < 100.0 >

6 FACTOR Relaxation factor to prevent divergence < 0.8 >

Block-4 /NRMAX/

NK(*i*) Number of mesh intervals by region (*i*)

Block-5 /NRMAX/

IK(*i*) Material number by region (*i*); the material number is assigned by the order of the material appears in the material specification (cf. Sect.2.9.)

Block-6 Required even if NXR=0 /NRMAX/

IXR(*i*) X-Region number by region. Enter all 0, if not necessary

Block-7 /NRMAX/

RK(*i*) Outer radii (distance from the origin) by region in cm.

Block-8 /1/

BSQ Transverse buckling B^2 in cm^{-2}. Neutron leakage is taken into account by pseudo absorption as $\Sigma_{a,g}^{eff} = \Sigma_{a,g} + D_g B^2$

Block-9 Required if IBOUND=2 /1/

XLAMD Group-independent constant for the extrapolation distance. For the Milne's problem XLAMD corresponds to 0.4692. The larger value gives shorter extrapolation distance. (cf. XMIS1 of Card-003-4 in Sect.2.8)

2.8 CITATION ; Multi-Dimensional Diffusion Calculation

The input of this section is required if IC2=5 or IC12=5 is specified in Sect.2.2 for the execution of CITATION routine. The requirement keeps the original input format[6] so that the same input data except the leading Blocks and final two Blocks can be used in separate execution of the original CITATION code. The description below uses the term 'Card' instead of 'Block' for the input data which are the same as original CITATION. The input data belonging to Card must be entered in the fixed column format as in the original CITATION.

Several additional functions are available as seen in the leading Block specifications such as the perturbation calculation, the application of anisotropic diffusion coefficients, the material dependent fission neutron spectrum, and the calculations of the generation time and the effective delayed neutron fraction, while several functions in the original CITATION are suppressed.

The CITATION can treat 12 types of models of one-, two- or three-dimensional geometries as shown in Table 2.8-1. The input requirements are explained by using mainly models on Cartesian coordinates (X-Y-Z coordinates), and other geometrical models correspond as shown in this table. Attention should be paid to R-Z model, where the vertical direction is treated as Y-direction in the CITATION.

Table 2.8-1 Geometries in CITATION and their correspondences to X-Y-Z model

Geometry model	X (column)	Y (row)	Z (plane)
1 D slab	X		
1 D cylinder	R		
1 D sphere	R_S		
2 D slab	X	Y	
2 D cylinder	R	Z	
2 D circle	θ	R	
2 D hexagonal	X_H	Y_H	
2 D triangular	X_T	Y_T	
3 D slab	**X**	**Y**	**Z**
3 D cylinder	θ	R	Z
3 D hexagonal	X_H	Y_H	Z
3 D triangular	X_T	Y_T	Z

In the CITATION, the terms 'zone', 'region' and 'mesh' are used as spatial disposition. A zone is a unit to allocate a material (cross-section) and also is used as a spatial unit to edit neutron flux and power distribution. A region is a geometrical unit defined by coordinates specified by the input data. A zone consists of one or more region(s). A mesh is a subdivision of a region. As the finite differential

equation is applied to meshes, the accuracy of solution depends on mesh size. For typical geometrical models, they are illustrated at the end of this section so that the user can understands the relation among zone, region and mesh.

The terms ‘left’, ‘right’, ‘top’, ’bottom’, ‘front’ and ‘back’ are used to indicate boundary surfaces (or directions) of three-dimensional space under consideration. Figure 2.8-1 shows them on X-Y and X-Y-Z models, and they are applied to all other models by the correspondence in Table 2.8-1. Note that the ‘top and bottom’ in CITATION is inverse positioning to that of TWOTRAN.

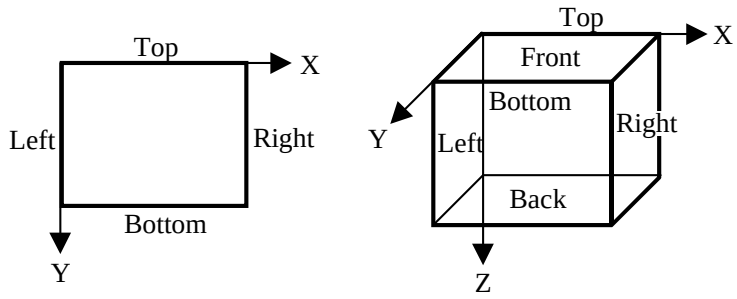


Fig.2.8-1 Naming of boundary surfaces in CITATION

Block-1 Control integers, always required /3/

1 NM ±Number of zones

As a special case, the number NM dose not count the zone allocated to the internal black absorber whose cross-sections are not defined. See NUAC17 in Card-003-2 and XMIS2 in Card-003-4.

Negative value activates the entry of the linear perturbation theory calculation specified by Block-4 through Block-8.

2 NXR Number of X-Regions to make homogenized flux and cross-sections in PDS files. Enter 0 if it is not required.

3 ID Option to select diffusion coefficient (cf. IC17 in Sect. 2.2)

= ±1 Select D1 in the SRAC macroscopic format through the CITATION routine

= ±2 Select D2

= ±3 Select D1 or D2 for the particular direction specified by the following Block-3 by material.

Negative value activates the entry for the calculations of the material dependent fission neutron spectrum and/or the effective delayed neutron fraction.

Block-2 Additional control integers required if ID<0 /2/

1 IXKI Option to prepare the material dependent fission neutron spectrum χ.

= 0 Unique spectrum is used (the spectrum of the fissile material which appears first in the material specification will be used).

= 1 Spectrum by material will be used (recommended).

2 IDELAY Option to calculate one-point kinetics parameters (effective delayed neutron fraction, generation time, etc.)

= 0 Skip

= 1 Calculate

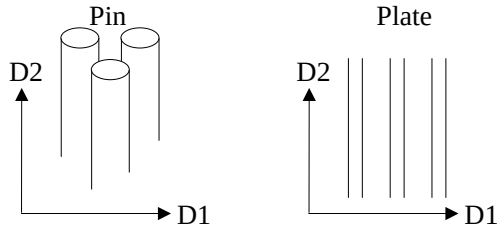
If IDELAY=1 is specified, the calculation of adjoint flux is required. Do not forget to specify non-zero value to NGC12 in Card-001-2 to activate the adjoint flux calculation.

Block-3 Required if ID=±3 is specified /NM/

IXYZ(*i*) Selection of directional diffusion coefficients by Zone (*i*),

IXYZ	D_X	D_Y	D_Z
=1	D1	D1	D1
=2	D2	D1	D1
=3	D1	D2	D1
=4	D2	D2	D1
=5	D1	D1	D2
=6	D2	D1	D2
=7	D1	D2	D2
=8	D2	D2	D2

The values on D1, D2 depend on the specification of IC17 (Sect.2.2) in the case where the cross-sections were formed. When IC17=±3 was specified the following directional diffusion coefficients are preserved;



In cylindrical geometry, D1 for radial and D2 for axial direction, and in slab geometry, D1 for across plane direction and D2 for parallel direction are stored.

In one- or two-dimensional calculation, the diffusion coefficients used for the transverse leakage term together with the buckling values entered in Card-024 are taken from D_Z.

The hexagonal model has the third boundary surface in addition to X- Y-directions on the plane. The leakage from the third surface is evaluated by D_X and the result is included into the leakage of X-direction (right and left).

Block-4 Control for perturbation calculation, required if NM<0 /1/

ICASE Number of cases for perturbation calculation after a CITATION calculation. If ICASE>0, do not forget to specify NGC12 in Card-001-2 to activate the adjoint flux calculation.

Repeat Block-5 through Block-8 ICASE times, required if ICASE>0

Block-5 /A8, 2, 1/

1 SAMPLE Member name (A8) of the macroscopic cross-section to be used in the perturbed region. Deviation of cross-sections from those unperturbed is automatically calculated.

2 IOPT Option to specify the perturbed region

= 1 Region is specified by the mesh intervals given in Block-6.

= 2 Region is specified by the X-Y-Z abscissa given in Block-7.

= -*N* Whole regions in the *N*-th zone

3 IDOPT Selection of the diffusion coefficients of the member SAMPLE

= 1 Use D1 for all direction ($D_X=D_Y=D_Z=D1$)

=	2	Use D2 for all direction	(D_X=Dy=D_Z=D2)
=	3	Use D1 and D2 as	(D_X=D2, D_Y=D1, D_Z=D1)
=	4	Use D1 and D2 as	(D_X=D1, D_Y=D2, D_Z=D1)
=	5	Use D1 and D2 as	(D_X=D2, D_Y=D2, D_Z=D1)
=	6	Use D1 and D2 as	(D_X=D1, D_Y=D1, D_Z=D2)
=	7	Use D1 and D2 as	(D_X=D2, D_Y=D1, D_Z=D2)
=	8	Use D1 and D2 as	(D_X=D1, D_Y=D2, D_Z=D2)

The coefficient for the pseudo leakage term (DB^2) uses always D_Z.

4 BKLE1 Buckling value (cm^{-2}) for the perturbed region

≥ 0.0 Constant buckling over whole energy groups

< 0.0 Floating number of groups. Group dependent buckling values will be read by Block-8.

Block-6 Required if IOPT=1 /6/

Region specification by mesh intervals

IXYZ(1,1) X-mesh interval number of the left side boundary

IXYZ(2,1) X-mesh interval number of the right side boundary

IXYZ(1,2) Y-mesh interval number of the top side boundary

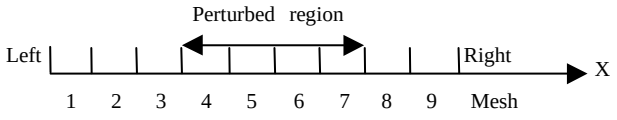
IXYZ(2,2) Y-mesh interval number of the bottom side boundary

IXYZ(1,3) Z-mesh interval number of the front side boundary

IXYZ(2,3) Z-mesh interval number of the back side boundary

Note:

Even one- or two-dimensional calculation requires 6 entries, feed zero values if not significant.



IXYZ(1,1)=4, IXYZ(2,1)=7

Block-7 Required if IOPT=2 /6/

Region specification by X-Y-Z abscissa.

XYZ(1,1) X-abscissa of the left side boundary

XYZ(2,1) X-abscissa of the right side boundary

XYZ(1,2) Y-abscissa of the top side boundary

XYZ(2,2) Y-abscissa of the bottom side boundary

XYZ(1,3) Z-abscissa of the front side boundary

XYZ(2,3) Z-abscissa of the back side boundary

Note:

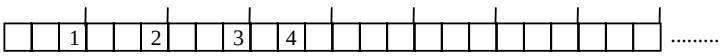
Even one- or two-dimensional calculation requires 6 entries, feed zero values if not significant.

The boundary abscissa is not necessarily coincided with mesh boundary. If any abscissa coincides with the abscissa of the original mesh point, enter negative floating number of the mesh interval number. It is to avoid the truncation error to compare two almost equal floating numbers.

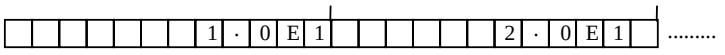
Block-8 Required if BKLE1<0.0 in Block-5 /BKLE1/

BKLE(*i*) Group(*i*) dependent buckling values (cm^{-2}).

The data starting at Card-Title-1,-2, Card-001, 003,…. through Card-999 have the same organization as the original CITATION. For these data, free format of the SRAC is not available, and the user must enter input by the fixed column format. Some old FORTRAN compilers may regard the following integers as 1, 2, 3, and 40 in the fixed format (24I3).



The floating numbers below may be regarded as 1.0E+1 and 2.0E10 in the format (6E12.5).



Card-Title-1 Comment (1) for calculation /A72/

Card-Title-2 Comment (2) for calculation /A72/

========== Section 001 : General Control ==========

Card-001-1 Section name (I3)

Enter ’001’

Card-001-2 Control options (24I3)

NGC1 Depletion option

= 0 (suppressed)

NGC2 Restart option

= 0 No restart.

= -1 Continue a previous case.

> 0 Restart a depletion calculation (suppressed)

Note:

To exercise a restart, a complete set of data must be supplied for the Section 001. When NGC2 $\neq$ 0, a restart file properly written from earlier machine run must be prepared by NGC3 below.

NGC3 Option to write restart data to permit restart

= 0 Skip

> 0 Write on logical device 13

NGC4 = 0 (not used)

NGC5 Option to save macroscopic cross-sections

= 0 (suppressed)

NGC6 Option to write neutron flux map

= 0 Skip

= 1 Write on I/O logical device 9

The flux (n/cm^2-sec) written on logical device 9 can be read by the following FORTRAN statements;

----- For 1-D or 2-D problem -----

```
DOUBLE PRECISION FLX2D(MX,MY,NG)
REWIND 9
DO IG=1,NG
  READ(9) ((FLX2D(IX,IY,IG),IX=1,MX),IY=1,MY)
END DO
```

--- For 3-D problem ---

```
DIMENSION FLX3D (MX,MY,MZ,NG)
DIMENSION WORK (MX*MY*MZ*NG)
EQUIVALENCE (FLX3D(1,1,1,1), WORK(1))
NDATA = MX*MY*MZ
REWIND 9
DO IG=1,NG
  J = (IG-1)*NDATA
```

```
      READ(9) (WORK(J+I),I=1,NDATA)
    END DO
```

where MX, MY, MZ, NG are number of mesh points on X-, Y-, Z-direction and number of groups, respectively.

NGC7 Option to write mesh information and mesh-wise power density distribution

= 0 Skip

= 1 Write on I/O logical device 32

The power distribution (W/cm^3) written on logical device 32 can be read by the following FORTRAN statements;

```
      DIMENSION POWER(MAXX,MAXY,MAXZ)
      REWIND 32
      READ(32) (TITL1(I),I=1,18), (TITL2(I),I=1,18),
     & IGEOM,MX,MY,MZ,NGC21,NGC7,
     & (X(IX),IX=1,MX),(Y(IY),IY=1,MY),(Z(IZ),IZ=1,MZ)
      READ(32) DUM,TOTP,AKEFF
      READ(32) (((POWER(IX,IY,IZ),IX=1,MX),IY=1,MY),IZ=1,MZ)
```

where MX, MY, MZ are number of mesh points on X-, Y-, Z-direction, respectively.

NGC8 Option to write mesh-wise neutron source (space-energy) on logical unit 17 (See GLIM5 in Card-001-5)

= 0 Skip

= 1 Write on I/O logical device 17

The neutron source distribution (n/sec) written on logical device 17 can be read by the following FORTRAN statements;

```
      DIMENSION S (MX,MY,MZ,NG)
      REWIND 17
      DO 100 IG=1,NG
        READ(17) (((S(IX,IY,IZ,IG),IX=1,MX),IY=1,MY),IZ=1,MZ)
  100 CONTINUE
```

where MX, MY, MZ, NG are number of mesh points on X-, Y-, Z-direction and number of groups, respectively.

NGC9 = 0 (not used)

NGC10 Problem type

= -5 Fixed source mode by IC2=5 or external source problem by IC12=5 with

source fed by Card-026.

= 0 Effective multiplication factor (k_{eff}) calculation

NGC11 Search option

= 0 (suppressed)

NGC12 Option for adjoint flux calculation

= 0 Skip

= ±1 Calculate adjoint flux. If negative, the adjoint flux will be printed out.

For the calculation of kinetic parameters β_{eff}, Λ or a perturbation calculation, enter NGC12=±1.

NGC13 Option to input the adjoint flux

= 0 Skip

= 1 The adjoint fluxes are read from logical unit 28.

= -1 Both of the forward and adjoint are read from logical unit 28

In this case, all input data are required as if the fluxes are newly calculated.

NGC14 = 0 (not used)

NGC15 Termination option

= 0 Terminate calculation and proceed as if converged if machine time or iteration count is exceeded (See Card-001-4).

= 1 If limits are exceeded, terminate calculation and proceed as if converged only if the iterative process is converging.

= 2 If limits are exceeded, terminate calculation.

NGC16 = 0 (not used)

NGC17 = 0 (not used)

NGC18 Residue calculation option

= 0 Values of the multiplication factor and the relative macroscopic

absorption cross-section, each of which minimizes the sum of squares of the residues of the point neutron balance equations, are obtained after termination of each eigenvalue problem.

< 0 This calculation is not done.

NGC19 = 0 (internally set)

NGC20 = 0 (not used)

NGC21 = 0 (suppressed)

NGC22 = 0 (suppressed)

NGC23 = 0 (ineffective)

NGC24 = 0 (not used)

Card-001-3 Edit options (24I3)

In the description below, the option will be exercised if the input number is > 0.

IEDG1 Print iteration information.

IEDG2 = 0 (suppressed)

IEDG3 Print macroscopic scattering cross-sections

IEDG4 Print macroscopic reaction rate cross-sections

IEDG5 Print gross neutron balance over system by group

IEDG6 Print gross neutron balance by zone by group

IEDG7 = 0 (suppressed)

IEDG8 = 0 (suppressed)

IEDG9 Print zone average flux values by group

IEDG10 Print point flux values by group

IEDG11 = 0 (not used)

IEDG12 Print zone average power densities

IEDG13 Print relative power density traverses through peak

IEDG14 Print mesh-wise power densities

IEDG15 = 0 (suppressed)

IEDG16 Print mesh-wise neutron densities summed over energy

IEDG17 = 0 (suppressed)

IEDG18 though IEDG23

= 0 (ineffective)

IEDG24 Option added on SRAC-CITATION

= 0 Print zone placement on fine mesh

= 1 Suppress printing of zone placement on fine mesh.
This is effective for saving too many pages printing for 3D case.

Card-001-4 General iteration count and machine time limits (24I3)

Problems are terminated when the iteration count reaches the limit and the calculation proceeds as specified by NGC15 in Card-001-2. As SRAC treats a static problem (no depletion or dynamics) only ITMX1, ITMX19, and ITMX24 are applied.

Built-in numbers are shown in < >; zero input data are replaced by these.

ITMX1 The limit of the iteration count <200>

ITMX2 through ITMX18

= 0.0 (ineffective)

ITMX19 The upper limit of CPU time (min) for an eigenvalue calculation <60>

ITMX20 through ITMX23

= 0.0 (ineffective)

ITMX24 The upper limit of total CPU time (min) for CITATION calculation <120>
This time does not include CPU time elapsed before and after CITATION calculation.

Card-001-5 General restraints (6E12.5)

Any calculation will be terminated if the restraints of GLIM1 and GLIM2 are not met. Built-in numbers are shown in < >; zero input data are replaced by these.

GLIM1 Maximum multiplication factor <1.5>

GLIM2 Minimum multiplication factor <0.5>

GLIM3 = 0.0 (suppressed)

GLIM4 = 0.0 (not used)

GLIM5 Factor applied to neutron productions for generating a fixed source file, see NGC8 <1.0>

GLIM6 = 0.0 (suppressed)

========== Section 003 : Description of the neutron flux problem ==========

Card-003-1 Input section name (I3)
Enter ’003’.

Card-003-2 General description (24I3)

NUAC1 = 0 (not used)

NUAC2 Initialization of the flux for a restart calculation (effective if NGC2= -1)

= 0 Use available flux, multiplication factor and acceleration parameters from

the previous problem

= 1 Use only flux from a previous calculation

= 2 Use built-in initialization procedure.

This number should be always 0 in SRAC, because only the continuation of a static problem (NGC2<0) is supported.

NUAC3 = 0 (not used)

NUAC4 = 0 (not used)

NUAC5 Geometry option

= 1 One-dimensional slab (X)

= 2 One-dimensional cylinder (R)

= 3 One-dimensional sphere (R_S)

= 4 (not used)

= 5 (not used)

= 6 Two-dimensional slab (X, Y)

= 7 Two-dimensional cylinder (R, Z)

= 8 Two-dimensional circle (θ, R)

= 9 Two-dimensional hexagonal (X_H, Y_H)

= 10 Two-dimensional triangular (X_T, Y_T)

= 11 Three-dimensional slab (X, Y, Z)

= 12 Three-dimensional cylinder (θ, R, Z)

= 13 Three-dimensional hexagonal (X_H, Y_H, Z)

= 14 Three-dimensional triangular (X_T, Y_T, Z)

NUAC6 = 0 (not used)

NUAC7 = 0 (not used)

NUAC8 Indicator of two-dimensional diagonal symmetry on X-Y plane (on plates if 3-D). This item is for speedup of computation time.

= 0 Skip

> 0 There is symmetry about the diagonal starting at the upper left-hand

corner and there are the same number of rows and columns

< 0 There is inverted diagonal symmetry.
Set to 0 if NUAC11= -1

NUAC9 Indicator of two-dimensional symmetry along column slices (on X-Z plane) for 3-D problems only. This item is for speedup of computation time.

= 0 Skip

> 0 There is symmetry about the diagonal starting at the upper left-hand corner and there are the same number of rows and columns

< 0 There is inverted diagonal symmetry.

NUAC10 = 0 (not used)

NUAC11 Left boundary condition (always effective)

= -1 Periodic (implemented for geometries given by NUAC5= 1, 6, 8, 11 and 12, left to right boundary closure only)

= 0 Extrapolated

= 1 Reflected

NUAC12 Top boundary condition (effective for 2-D,3-D)

= 0 Extrapolated

= 1 Reflected

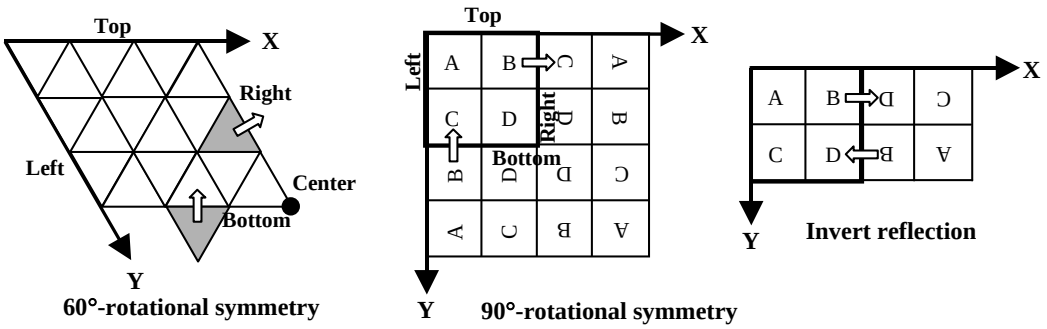
NUAC13 Right boundary condition (always effective),
Set to -1 if NUAC11= -1

= 0 Extrapolated

= 1 Reflective

= 2 90° rotational symmetry (slabs)
60° rotational symmetry (triangular)

= 3 Inverted reflection (180° rotational symmetry, slab only)



NUAC14 Bottom boundary condition (effective for 2-D, 3-D)

= 0 Extrapolated

= 1 Reflected

NUAC15 Front boundary condition (effective for 3-D)

= 0 Extrapolated

= 1 Reflected

NUAC16 Back boundary condition (effective for 3-D)

= 0 Extrapolated

= 1 Reflected

NUAC17 Option for internal black absorber

= 0 No internal black absorber

> 0 Zone number of internal black absorber

An internal black absorber has the logarithmic differential (non-return) boundary condition applied at its surfaces. This zone will be black to all groups unless additional data are supplied to certain groups) by XMIS2 on Card-003-4. The cross-sections given to the zone may be accepted to the specified groups. In this case, the slowing-down neutrons into the groups specified as black absorber are entirely absorbed. Only one zone is allowed as an internal black absorber.

NUAC18 Option to allow negative neutron flux

= 0 Negative flux is not allowed

> 0 Negative flux is allowed (suggested)

NUAC19 Override use of Chebychev polynomials in adjusting the parameters

= 0 Chebychev polynomials are used

> 0 Chebychev polynomials are not used

NUAC20 Line relaxation option

= -2 Apply on Y- and X-direction only

= -1 Apply on Y- X- and Z-direction alternatively

= 0 for the problem involving up-scattering, apply on Y-direction only with one inner iteration. If no up-scattering, on X- and Y- alternatively in 2-D problem, and at three inner iterations for 3-D problems without I/O and at five with data I/O during iteration

> 0 apply only on Y-direction

NUAC21 = 0 (not used)

NUAC22 = 0 (not used)

NUAC23 Specified number of inner iterations.

= 0 Use defaulted value

> 0 Specify the value

NUAC24 = 0 (not used)

Card-003-3 Iteration convergence criteria (6E12.5)

Built-in numbers are shown in < >; zero input data are replaced by these.

EPSI1 Maximum relative flux change for the last iteration <0.0001>

EPSI2 Maximum relative change in the eigenvalue for the last iteration <0.00001>

EPSI3 = 0.0 (not used)

EPSI4 = 0.0 (ineffective)

EPSI5 = 0.0 (not used)

EPSI6 = 0.0 (not used)

Card-003-4 Miscellaneous data (6E12.5)

XMIS1 External extrapolated boundary constant C_g

> 0 The constant for all extrapolated boundaries (See NUAC11-16) for all groups

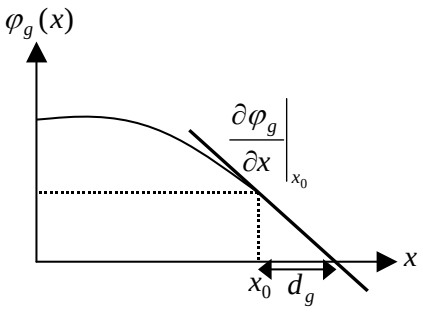
< 0 This is the total number of energy groups and Card-003-5 are to follow this card, which give the group-dependent extrapolated boundary constants for problem boundaries for all energies.

= 0 The code will use the built-in value for all extrapolated boundaries <0.4692>

Note:

The extrapolated boundary constant C_g of energy group g is defined as

$$C_g = \left[\frac{-D_g}{\varphi_g} \frac{\partial \varphi_g}{\partial x} \right]_{X=X_0}$$



and as the extrapolated length d_g is defined by

$$\frac{1}{d_g} \equiv \left[\frac{-1}{\varphi_g} \frac{\partial \varphi_g}{\partial x} \right]_{X=X_0}$$

thus the relation $C_g = D_g/d_g$ holds, where D_g is diffusion coefficient.

As the diffusion coefficient D_g is defined as

$$D_g = \frac{1}{3\Sigma_{tr,g}} = \frac{\lambda_{tr,g}}{3},$$

the constant C_g has the relation below;

$$C_g = \lambda_{tr,g} / 3d_g$$

If the extrapolation length of the Milne's problem $d_g = 0.7105\lambda_{tr,g}$ is applied, the extrapolation constant C_g becomes the defaulted value (0.4692) which does not depend on neutron energy. It is the reason to apply XMIS1=0.0 (defaulted value for all groups). If a sufficiently large value of extrapolation constant is applied, $d_g=D_g/C_g$ tends to zero so that the zero flux at the boundary is assumed.

XMIS2 The extrapolation constant for internal black absorber boundary specified by

NUAC17

> 0 The constant for all groups applying to zone NUAC17

< 0 This is the total number of groups (negative) and Card-003-6 is to follow, after any required above, which gives the internal black absorber boundary constants for each energy group. Zero value indicates that the black absorber boundary condition is not applied to that group. (flux is calculated with given cross-sections, e.g. for fast group).

= 0 The code will use the built-in value for all groups and the absorber will be black over all energy <0.4692>

Note:

For the case that involves strong absorber like control rod where the diffusion theory can not be applied, the internal black absorber may be introduced. The extrapolation constant is given by the comparison with the results of a transport calculation or/and experiments. If the cross-sections are used for certain groups, specify XMIS2<0.0. (See Card-003-6).

XMIS3 Core power level in MWt

> 0 This value is used to normalize the power distribution and flux level.

= 0 Defaulted value <1.0> is used.

Note:

For 1-D or 2-D calculation, give the thermal power by assuming the whole core of unit length (cm) for the transverse direction(s). For example, to the X-Y calculation of the core with thermal power 3,000MWt in the effective core height 100cm, give XMIS3 = 3000/100 = 30.

XMIS4 Fission to power Conversion factor

> 0 Ratio of thermal energy to fission energy (XMIS3 is divided by this) Normally set 1.0.

= 0 Defaulted value <1.0> is used

XMIS5 Core symmetry factor

The thermal power given by XMIS3 are divided by this number.

> 0 Core symmetry factor i.e. fraction of the core considered; e.g. for 1/4 symmetric core, enter XMIS5=0.25

= 0 Defaulted value <1.0> is used

Note:

e.g. In the 3-D 1/4 symmetric core calculation, enter XMIS5=0.25, if XMIS3=3,000 is given as whole core power. In the same case, enter XMIS5=1.0, if XMIS3=3000*0.25= 750 is given.

XMIS6 Initial over-relaxation factor

> 0 Input value is used

= 0 Defaulted value <1.0> is used

Card-003-5 Required if XMIS1<0 (6E12.5)

The extrapolated boundary constants for problem boundaries. For 1-D problems, beginning with those for all energies for the left boundary, then data are required for the right boundary by starting with a new card. For 2-D, give the constants in the order left, top, right and bottom by a new card for each boundary. For 3-D problems, give them for six boundaries in the order left. top, right, bottom, front and back.

For the periodic boundary condition, NUAC11=-1, skip the left and right boundaries. For 90° rotational symmetry, NUAC13=2, skip the right and bottom. For 180° rotational symmetry, NUAC13=3, skip the right. Even the reflective condition is specified for the left, enter the constants of value 0.0.

Card-003-6 Required if XMIS2<0 (6E12.5)

The internal black absorber boundary constants for each energy group. Zero value indicates that the black absorber boundary condition is not applied to that group. (flux is calculated with given cross-sections, e.g. for fast group).

========== Section 004 : Geometric mesh description ==========

Card-004-1 Input section name (I3)

Enter ’004’

Card-004-2 6(I3,E9.0)

Specify the number of mesh points and the region width for each vertical region going from left to right. For a two-dimensional problem also specify the number of mesh points and the region width for each horizontal region going from the top to

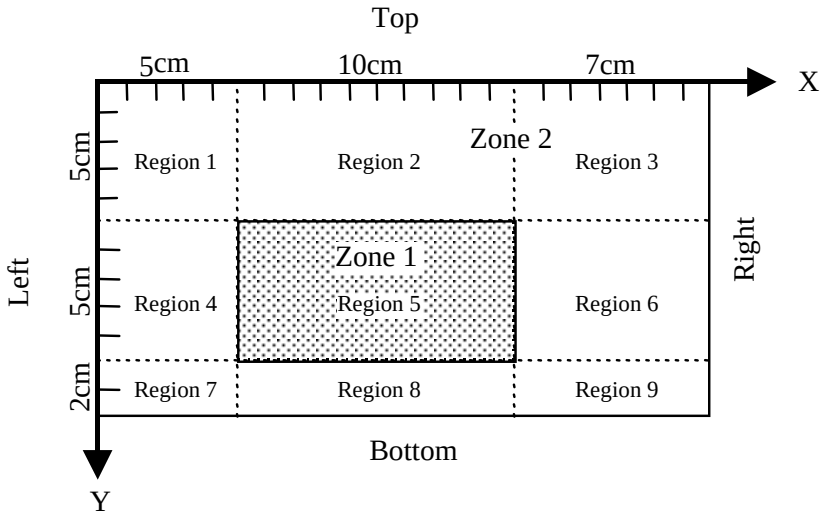
bottom starting with a new card. For a three dimensional problem also specify the number of mesh points and the region width for each region going from front to back.

In referring to the geometric mesh, rows of mesh points go from top to bottom, column of mesh points go from left to right, and planes of mesh points go from front to back. In R and R-Z geometry, a row is a radial traverse. in θ-R and θ-R-Z geometries, columns radiate downward from a center at the top and a row has constant radius. In hexagonal and triangular geometries the X and Y are assumed to be at 60° (upper left-hand corner), and dimensions are on external boundaries; these treatments are precise only if points on any plane have equal finite-difference volumes.

Data must be ended for each traverse by a blank entry; if the last card of data is filled for any traverse (number of entries is a multiple of 6), another blank card is required.

Region width is specified in cm, and in θ-R and θ-R-Z geometries, θ width is entered by a radian unit to make 360° to 2π.

Mesh is sub-divided to make equal size, while radial direction is sub-divided to make equal volume.



For the above two-dimensional case assuming all mesh intervals are 1 cm, input data are given as:

```
---------+---------+---------+---------+-----
004
  5        5.0 10      10.0  7       7.0  0
  5        5.0  5       5.0  2       2.0  0
---------+---------+---------+---------+-----
```

========== Section 005 : Zone placement ==========

Card-005-1 Input section name (I3)

Enter ‘005’.

Card-005-2 (24I3)

Allocate the zone identification numbers of each vertical region. The order of input is for the first horizontal row of regions going from left to right. For a one-dimensional problem the zone numbers are specified for only horizontal regions.

For 2-D problem, beginning with a new card, specify the zone numbers of each vertical region in the second horizontal row of regions. Continue these specifications going from top to bottom.

A sample input for Card-005 is as follows:

```
---------+---------+---------+---------+-----
005
  2   2   2
  2   1   2
  2   2   2
---------+---------+---------+---------+-----
```

For a three-dimensional problem, give the two-dimensional grid for each block of mesh-point planes going from front to back.

========== Section 006 : Mesh overlay ==========

New zones may be superimposed within a mesh described with this data. But the input of this section is not necessarily required. Zone number allocation by region given by 005 section is internally replaced by code into zone number allocation by mesh. This zone allocation by mesh can be replaced with this data.

e.g. if a map of a core with the control rod withdrawn is described by 005 section, zone number of the meshes where the control rod is inserted can be modified by using 006 section. Thus, fine position of control rod insertion can be specified.

Card-006-1 Input section name (I3)

Enter ‘006’.

Card-006-2 Zone number (I3)

Repeat Card-006-2 and Card-006-3 until zero zone number (blank card) is encountered.

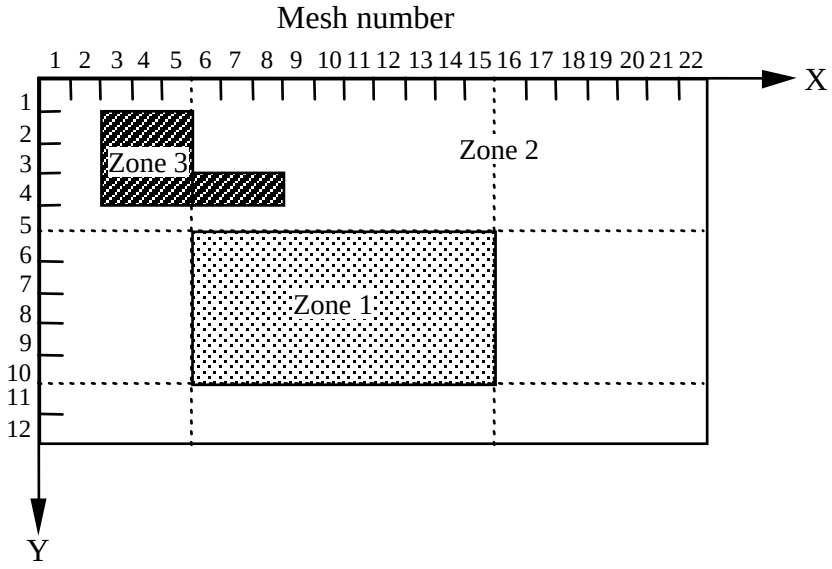
Card-006-3 Specification of meshes to superimpose 3(6I4)

Specify blocks of points by left column number and then right column number to give limits along rows, top and bottom row numbers for column limits, and front and back plane numbers for depth limits in that order. If only one row is involved, for example, then that row is repeated as limits. Only 4 entries among 6 are valid for each specification in 2-D geometry. Data is read until zero value is encountered on the first column number. The entry ‘000600060005001500020002’ places the new material along column 6 from row 5 through 15 and on plane 2 only.

Remember that each mesh point has an associated volume around it (as mesh points do not lie on material interfaces); specifying a single mesh point here, say ‘000600060005000500020002’ does involve an associated volume.

A sample to specify Zone 3 as overlay area in the below 2-D model

```
---------+---------+---------+---------+-----
006
   3
   3    5    2    4    0    0    6    8    4    4    0
   0
---------+---------+---------+---------+-----
```



========== Section 008 : Macroscopic cross-sections ==========

Macroscopic cross-sections are supplied by two options. One is to read from this section described below (KMAX>0). The other is to read from an I/O unit (logical 31) where the form of the

data is identical with that of this input section. The CVMACT routine in SRAC converts the data before calling CITATION by reading the data from PDS (MACRO or MACROWRK) file and writes them into logical unit 31. For the latter, Card-008-1 is required and then Card-008-2 containing a negative integer in columns 1-3 (KMAX<0), which complete the data for this section. Otherwise (KMAX>0), input data after Card-008-3 are required. We shall describe this section to explain the contents of the I/O unit 31.

Card-008-1 Input section name (I3)
Enter '008'.

Card-008-2 Number of groups and scattering range (3I3)

1 KMAX Number of energy groups
- < 0 Use the cross section provided by SRAC: Cross-sections are read from logical unit 31. As KMAX is automatically supplied on logical unit 31, absolute value of KMAX may be arbitrary.
- > 0 User's own cross-sections are read in this section, the KMAX value must be proper.

2 IX28 Number of groups for down-scatter
As the code finds the correct value from the scattering vector, this value may be different from the actual value.

3 IX29 Number of groups for up-scatter
As the code finds the correct value from the scattering vector, this value may be different from the actual value.

If KMAX<0, input for section 008 is completed.

Card-008-3 Cross-sections (2I6,5E12.5)

1 M Zone number

2 K Group number (g)

3 SIG1 Diffusion coefficient (D_g)

4 SIG3 Absorption cross-section ($\Sigma_{a,g}$)

5 SIG4 Production cross-section ($\nu\Sigma_{f,g}$)

6 SIG5 Constant ($\Sigma_{\upsilon,g} \equiv 1/\sqrt{\overline{E}_g}$) related on neutron velocity for the calculation of point kinetics parameters (cf. Sect. 3.1.5).

7 SIG6 Power per unit flux, (joule/fission)* $\Sigma_{f,g}$ for normalization of the flux level and power density maps. If all entries here are zero, then SIG4 is used. If KMAX<0, SIG6=3.246E-11* $\Sigma_{f,g}$ is filled by SRAC assuming the fission by U-235.

Card-008-4 Scattering cross-sections (6E12.5)
Specify the cross-section for scatter from group K (above) to each of the other groups 1 to KMAX. ($\Sigma_{K\rightarrow g'}$, g'=1,KMAX).

The code continues reading Card-008-3 and Card-008-4 until M=0 is found (blank card).

Card-008-5 Standard fission spectrum (6E12.5)
These values are common for all zones (χ_g ,g=1,KMAX)

For the functions peculiar to SRAC such as directional diffusion coefficients, material dependent fission spectra and kinetics parameter, further input data are required. As they are provided in logical unit 31 by SRAC, the explanation is omitted. If the functions are not used, input data for this section is complete.

========== Section 024 : Buckling specification ==========

Card-024-1 Input section name (I3)
Enter '024'.

Card-024-2 Indicator and buckling value (I3,E9.0)

1 IND Specification of buckling value

= 1 Specify a constant buckling in columns 4-12 (E9.0) on this card and no additional data is required.

= 2 Specify values of group dependent buckling starting with Card-024-4. In this case, the KMAX value in Card-008-2 must be proper.

= 3 Specify the group depending buckling to the set of consecutive zones specified on Card-024-3. In this case, the KMAX value in Card-008-2 must be proper. Continue with Card-024-3 and Card-24-4 for as many zones as required. A blank card (zero zone number) must be used to end this data.

2 BKLE Effective only if IND=1
Constant buckling value on columns 4 through12 in cm^{-2}

Card-024-3 Required if IND=3 (2I3)
Initial and final zone indicators; to the set of consecutive zones, the group dependent buckling on Card-024-4 will be applied.

Card-024-4 Required if IND=2,3 (6E12.5)
Group dependent buckling values

========== Section 026 : Fixed source specification ==========

The input of this section is required if the fixed source problem for the whole energy group is solved by specifying IC12=5 (Sect.2.2) and NGC1-=5 (Card-001-2). The solution does not converge in the system where the multiplication factor $k_{eff} \geq 1.0$.

Card-026-1 Input section name (I3)
Enter '026'.

Card-026-2 (2I3)

1 NFX1 Specification of fixed source

= -1 One spectrum of specified intensities into zones
Card-026-3 and Card-026-6 are required

= 0 One spectrum of specified intensities into specified mesh ranges
Card-026-3, Card-026-4 and Card-026-5 are required.

> 1 Read in from logical unit 17 the spatial distribution of source by group, They are read by the following FORTRAN statements

```
DIMENSION S(MX,MY,MZ,NG)
REWIND 17
DO IG=1,NG
  READ(17)(((S(IX,IY,IZ,IG),IX=1,MX),IY=1,MY),IZ=1,MZ)
END DO
```

2 NFX2 Optional print control

= 0 No print out of fixed source

> 0 Print out of fixed source

Card-026-3 Required if NFX1 ≤ 0 (6E12.5)

KMAX entries of relative values of source spectrum. Normalization to unity is not necessary. In this case, the KMAX value in Card-008-2 must be proper.

Card-026-4 Required if NFX1=0 (6I4,E12.5)

Specify blocks of points by left column number and then right column number to give limits along rows, top and bottom row numbers for column limits, and front and back plane numbers for depth limits in that order. If only one row is involved, for example, then that row is repeated as limits. Only 4 entries among 6 are valid for each specification in 2-D geometry. Data is read until zero value is encountered on the first column number. The entry '000600060005001500020002' defines the spatial range along column 6 from row 5 through 15 and on plane 2 only.

1 JL Left column number

2 JR Right column number

3 IT Top raw number

4 IB Bottom raw number

5 KBF Front plane number

6 BB Back plane number

7 X = 0.0 Give spatial distribution by Card-026-5

> 0.0 Use this value as a source intensity (n/sec-cm^3) over the spatial range specified above

Card-026-5 Required if NFX1=0 and X=0.0 (6E12.5)

Enter fine distribution of source intensity (n/sec/cm^3) in the range specified by Card-026-4 starting with the value at the left limit JL to the right limit JR on the horizontal raw IT, then those on the second raw until the raw limit IB on the plane KBF are met. Then data are required by beginning a new card for the second plane. The total number of entries is (JR-JL+1)*(IB-IT+1)*(KBB-KBF+1).

Repeat Card-026-4 and Card-026-5 until a blank Card-026-4 is encountered.

Card-026-6 Required if NFX1<0 (6(I3,E9.0)

Zone number and intensity (n/sec/cm^3) until zero zone number is encountered.

========== Section 099 : Termination of input ==========

Card-999-1 Input section name (I3)

Enter '999'.

Card-999-2 A blank card

A normal exit from the original CITATION routine may be affected by locating one blank card after Card-999-1 card. Here, the input for the second CITATION run can be placed before Card-999-1 card. However, the SRAC-CITATION routine allows only one set starting from Title cards until Card-999-2. After returning back to SRAC the second run of CITATION is available.

While the input format Card-001 through Card-999 is identical with that of the original CITATION, SRAC-CITATION requires further input for CITATION that is entered by the SRAC free format.

Block-9 Material specification /NM/

MAT(*i*) Material number by zone(*i*). This item is to select and to number the materials used in the CITATION routine from the materials listed in the material specification in Sect.2.9.

(MAT(*i*),*i*=1,NM), where NM is specified in Block-1.

Block-10 Required if NXR>0 specified in Block-1 /IZN/

NXREG(*i*) This item is to make the spatially averaged few-group cross-sections and/or flux.

(NXREG(*i*),*i*=1,IZN): X-Region number by region (*i*), IZN is the product of number of horizontal regions, that of vertical regions and that of planes for 3-D case.

The input instruction of SRAC-CITATION is over. The typical model examples are shown in Fig.2.8-2 through 2.8-7 for the convenience of users.

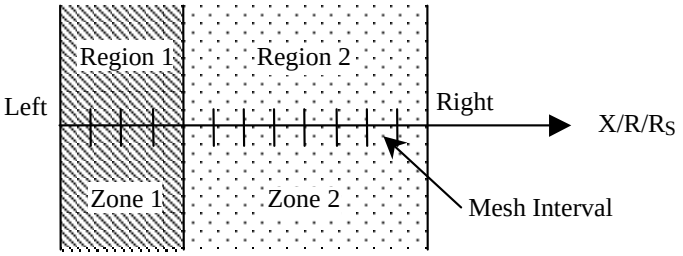


Fig.2.8-2 Sample geometrical model for 1D slab (X), 1D cylinder (R), 1D Sphere(Rs).

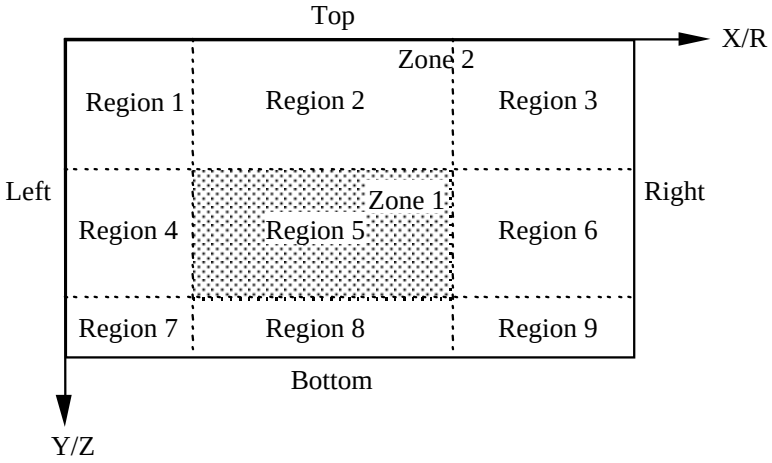


Fig. 2.8-3 Sample geometrical model for 2D slab (X-Y), 2D cylinder (R-Z).

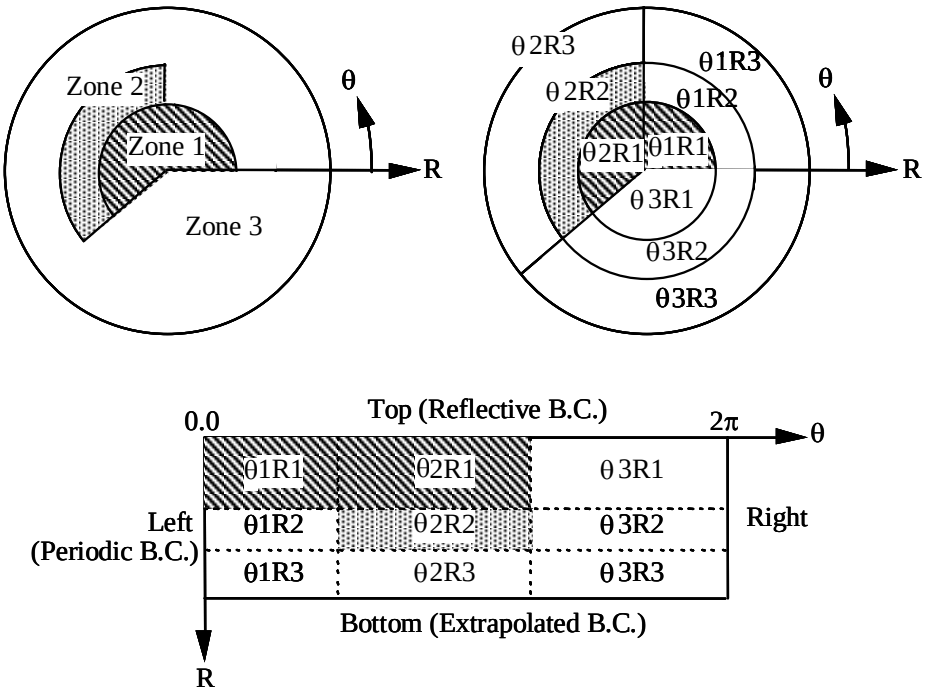


Fig. 2.8-4 Sample geometrical model for 2D circle (θ-R).

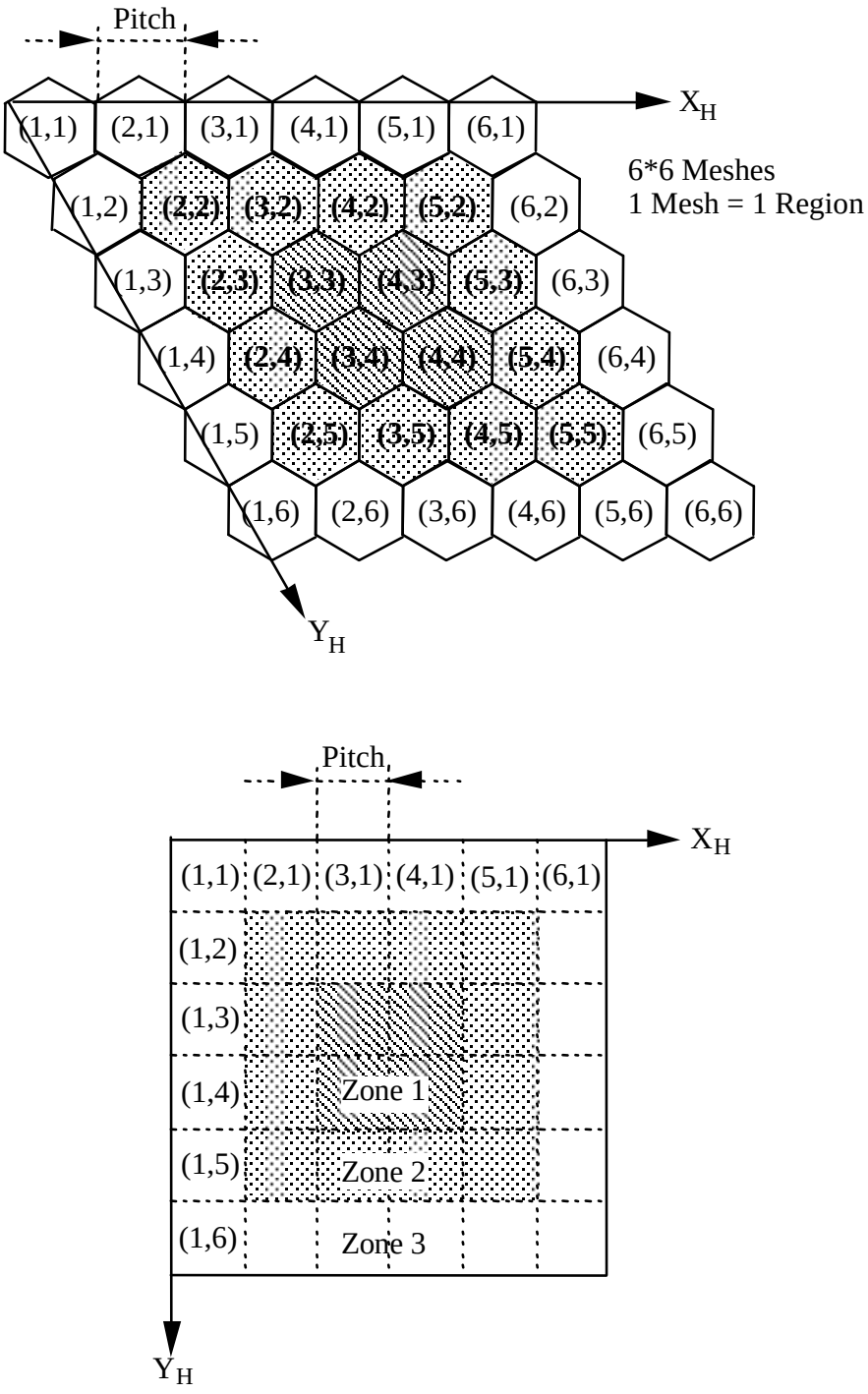


Fig. 2.8-5 Sample geometrical model for 2D Hexagonal (X_H-Y_H).

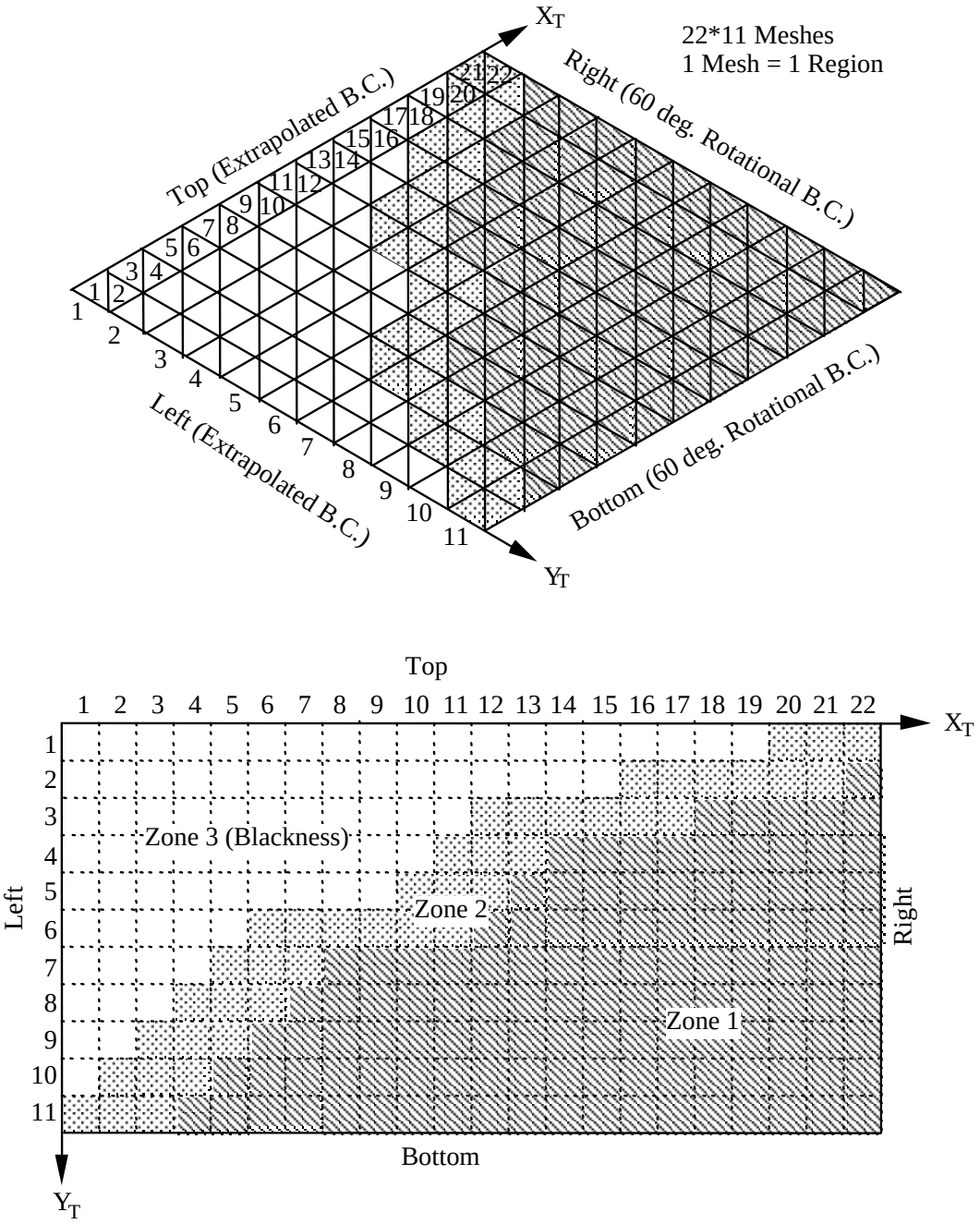


Fig. 2.8-6 Sample geometrical model for 2D Triangular (X_T-Y_T).

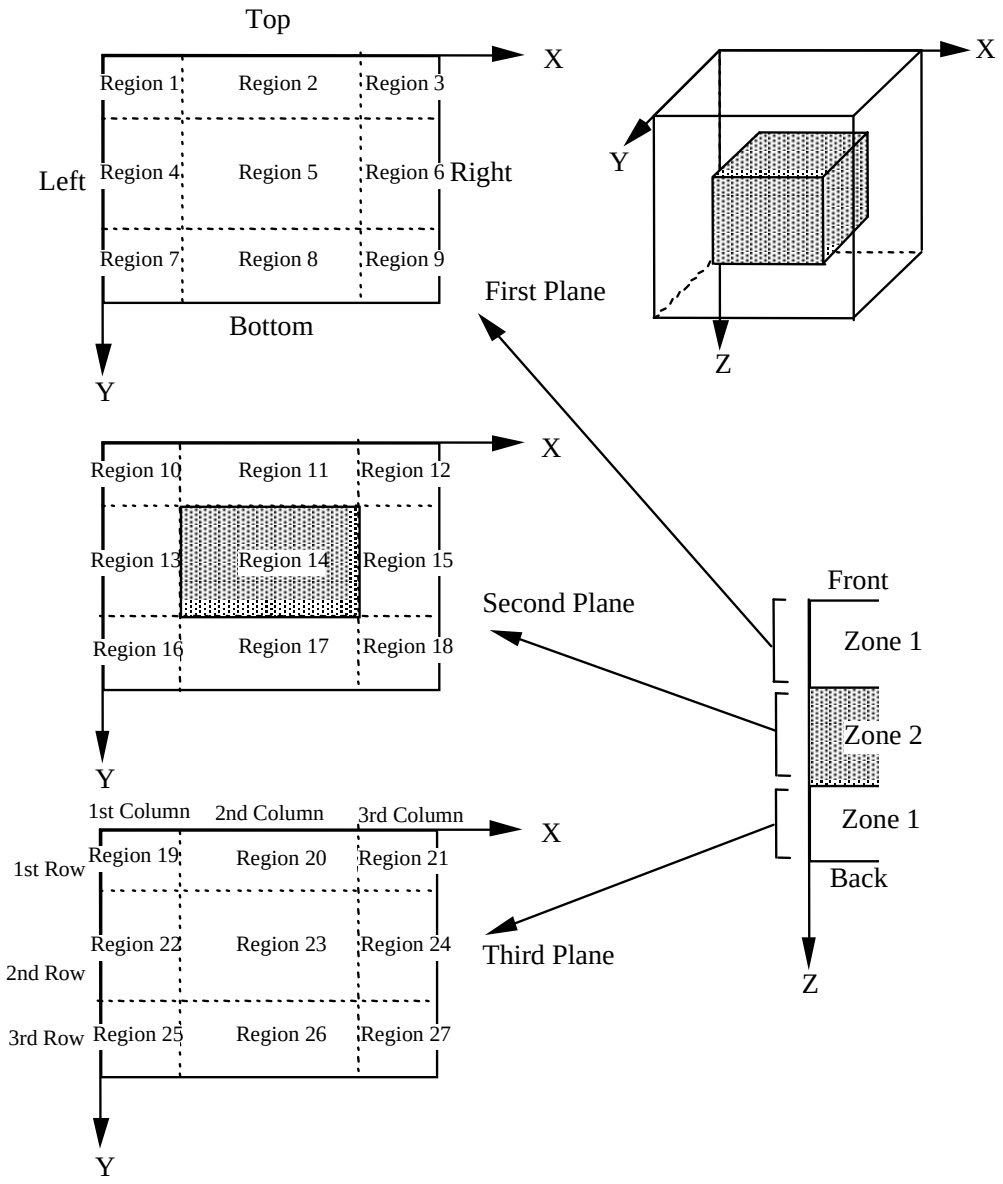


Fig.2.8-7 Sample geometrical model for 3D slab (X-Y-Z).

2.9 Material Specification

'Material' appearing in this section may be understood as it has a set of macroscopic cross-sections. Therefore, material name denoted by 8 characters expresses the name of material of which cross-sections are already on fine-group macroscopic cross-section file (MACROWRK) or few-group macroscopic cross-section file (MACRO) or will be formed. Several kinds of mixtures, as follows, are included in material.

- A mixture with composition to which macroscopic cross-sections will be formed in this case.
- A mixture of which macroscopic cross-sections were formed in the previous case and are kept in MACROWRK file. The composition is not given in this case.
- A homogenized material with a CASENAME label to which macroscopic cross-sections were formed in the previous case into MACROWRK and/or MACRO file. The former half of member name is the case name of the previous case.
- A homogenized material with the CASENAME label of this case to which macroscopic cross-sections are formed in this case, and will be used in the later step in this case or in the next case. If this material will not be used in this case, the material name does not appear in the material specification.
- A fictitious mixture with composition to be used only for reaction rate calculation.
- A fictitious mixture without composition of which macroscopic cross-sections were formed in the previous case into MACROWRK and/or MACRO file to be used only for reaction rate calculation.

Block-1 /1/

NMAT Number of materials to be specified hereafter.

Block-2 /A8, 2, 3/

1 MTNAME Material identification expressed by eight characters, composed of five tags as '*mmmm-e-b-x-p*' or '*case-e-b-x-p*' which appears as MEMBER name in macroscopic cross-section files.

mmmm-tag Material identification of 4 characters; the first character must be any alphabetic character.

case-tag To specify a set of X-Region averaged cross-sections formed in the previous case,

use the case name of the previous case. (e.g. CELL, TYP1, PWR1 etc.), together with *x*-tag.

Otherwise, *mmmm*-tag is used as the former half of member name on MACROWRK file to discriminate the member for a mixture. Therefore, do not use more than once the same *mmmm*-tag in a case. In a run of consecutive cases, if the same *mmmm*-tag appearing in the previous case is used in the succeeding case, even if the new composition is given, the formation of cross-sections is skipped and those formed in the previous case are used in the latter case. Exactly speaking, *x*-tag described later is also used for the discrimination. In this sense, the same *mmmm*-tag may be used for different mixtures.

e-tag — Tag internally used to specify the neutron energy range of a set of macroscopic cross-sections, because the sets for fast and thermal energy range are separately composed and later concatenated into the set for whole energy range. The code ‘F‘ for fast, ‘T’ for thermal, ‘A’ for whole energy range is assigned, respectively. The user can confirm it from the member list of MACROWRK file.

b-tag — Tag to indicate burn-up step as ‘0’ , ‘1’, ‘2’, ...,’9’ and ‘A’, ‘B’,...,’Z’, ‘a’, ‘b’, … and ’z’ corresponding to fresh, steps 1, 2.....,’9’ and 10, 11,..., 35, 36, 37, … and 61, respectively, when the cell burn-up calculation is done to make up this mixture. Otherwise this tag is filled by the character given in the input.
When the user wants to refer the cross-sections obtained in a series of burn-up calculations, he can specify the burn-up step by using this tag.

x-tag — *x*-tag has different function depending on whether the former half of member name is case name or mixture name.
Enter an alphameric character (1, 2,….,9, A, B, …) corresponding to X-Region number to specify an X-Region among a set of homogenized cross-sections formed in the previous case.
When a set of mixture cross-sections are newly formed by giving composition in this case, any character entered for this tag is used as the seventh character of the mixture name.
In the latter case, this tag is also used to discriminate the effective microscopic cross-sections stored in the MICREF file when a resonant nuclide is commonly used in more than one mixture. e.g., the microscopic cross-sections of ^{238}U in UO_2

fuel pin: MU08F0U2 and those in MOX fuel pin: MU08F0M2 on MICREF file are discriminated by the seventh character (*x*-tag=U or M). Therefore, the same *x*-tag should not be used for different resonant materials in a case or in consecutive cases.

p-tag Tag internally filled to specify Legendre component and also whether fine or coarse in energy group structure. Any character given in the input is replaced by the code.

= '0' coarse (few) and isotropic (with transport correction if by PIJ)

= '1' coarse and P_1 component (by S_N calculation)

= '2' fine and isotropic (with transport correction)

= '3' fine and P_1 component

= '4' fine and P_0 component

2 NCOM Enter NCOM=0 always (not used)

3 NISO Number of nuclides to compose the mixture (given by Block-3).
Enter NISO=0 to specify a set of cross-sections which were already formed into MACROWRK or MACRO file.
If the member specified by MATNAME exists already, even if NISO>0 and composition is given, formation of cross-sections is skipped and the old one will be used.

4 TEMP Physical temperature of the mixture in Kelvin (K).
Any temperature can be accepted for the interpolations of 1) the THERMAL library and 2) the resonance self-shielding factor, and 3) Doppler broadening of the Public MCROSS library, unless the extrapolation is required.

5 XL l ; the mean chord length of the resonance absorber lump used to include heterogeneous effect in the interpolation of resonance self-shielding factor in NR or IR approximation, and also used in PEACO for the constant to yield a non-dimensional blackness for the interpolations of the collision probabilities.
Generally l is defined as

$$l = 4\,V / S\,,$$

where V is the volume of the mixture, S is the surface area.

For a one dimensional slab of thickness *a*

$l = 2\,a$

For a one dimensional sphere of radius *a*

$l = 4\,a\,/\,3$

For a one dimensional cylinder of radius *a*

$l = 2\,a$

For a hollow cylinder of inner radius *a* and outer radius *b*

$l = 2\,b\,(\,1 - (\,a\,/\,b\,)^2\,)$

For more complicated geometry which contains several absorber lumps in a unit cell, enter the mean chord length of a dominant absorber, for example, to BWR lattice that of a pin rod.

6 DC — *C* ; the Dancoff correction factor (cf. Sec.1.6)

(effective only if IC3=0 in Block-3 of Sect.2.2 is specified)

If DC<0 is entered, Block-3' will be read instead of Block-3, which includes nuclide-dependent Dancoff correction factor.[19)]

Enter DC=1.0 for the homogeneous approximation. (no shadow effect)

Remind that *l* and *C* is used in a conventional table-look-up for the heterogeneous effect to the background cross-section σ_0 in the following form;

$$\sigma^i_{0,n} = \frac{1}{N^i_n}\sum_{m\neq n}(N^i_m\sigma^i_{t,m}) + \frac{g(C^i_n)(1-C^i_n)}{N^i_n l^i} \quad \text{for resonant material } (i) \qquad (2.9\text{-}1)$$

where $g(C)$ is a geometric correction factor to the simple NR approximation, *n* denotes the resonant nuclide under consideration and *m* any nuclide admixed in the material.

Block-3 — Required if NISO > 0 and DC ≥ 0 — NISO times /A8, 2, 1/

1 IDENT — Nuclide identification expressed by eight characters composed by seven tags '*X-zz-m-c*-b-*i-t*'. e.g. XH01H001 (H-1 in H_2O)

X-tag — Tag used internally to specify physical quantities, consequently any character is accepted in the input. Usually 'X' is entered.

zz-tag — Element symbol of the nuclide (cf. Sect.8.1)

Enter 'PU' for plutonium. For a nuclide denoted by one character such as H for

hydrogen, add character ‘0’ to complete the tag as ’H0’.

m-tag The last digit of the mass number is used to discriminate the isotopes as ‘9’ for Pu-239. ‘N’ is used to specify the element with natural abundance like ‘FEN’ for natural iron. A few exceptional cases occur when the excited states of some fission produced isotopes exist as PM-148-G and PM-148-M, and when there exist isotopes with the same last digit of the mass number like Sn-116 and Sn-126, where the special characters are used. Such special treatments and elements are listed in Sect.8.1

c-tag Chemical compound status tag to select the proper thermal scattering law (cf. Sect.8.1). Use ‘0’ for nuclide to treat with free gas model.
e.g. H01H for H in H_2O
When the effective microscopic cross-sections are written into MICREF file, this tag in the member name is internally set to ‘F’ or ‘T’ to select ‘fast’ or ‘thermal’ energy range.

b-tag Enter ‘0’ in usual input.

This tag is used internally for burn-up step indicator.
When the effective microscopic cross-sections are written into MICREF file while burn-up calculation is not carried, the sixth character of input data is used to this tag. To specify the data in MICREF file with IRES=1,enter the sixth character of the mixture name with which these effective cross-sections are associated.

i-tag Enter ‘0’ in usual input.

This tag is internally used to identify the material to which the effective microscopic cross-sections are associated.

To specify the effective microscopic cross-sections in MICREF file by setting 1 for the next item IRES, enter the seventh character of the mixture name to which the effective microscopic cross-sections are formed.

t-tag Temperature indicator (obsolete), any character is accepted.

This tag was used in the old version to specify the temperature on which data were tabulated. While this entry is ineffective as the interpolation is established,

this tag appears to denote the nearest temperature point to the material temperature as the 8-th character of the member for the effective microscopic cross-sections on MICREF file.

2 IRES Resonance cross-section process indicator.

= 0 Non resonant nuclide (or minor resonant nuclide whose heterogeneity is negligible)

To the resonant nuclide that has *f*-table based on the NR approximation, the interpolation of self-shielding factor will be done although the heterogeneous term $g(C)(1\text{-}C)/(N_n l)$ to evaluate the background cross-section σ_0 is not considered (C=1). The σ_0 is calculated for the homogenized system, if there is no resonant nuclide with IRES=2 in the material.

The IR approximation is not applied to this nuclide even if the resonance level parameters are installed.

= 1 Effective microscopic cross-sections, which have been calculated in the previous case, will be read from MICREF file as if this nuclide is non-resonant. (IRES=2, if double heterogeneity is considered) The member denoted by IDENT must exist on MICREF file.

= 2 Treatment as a resonant nuclide.

Effective microscopic cross-sections (before modification by IR or PEACO) is obtained by Eq.(2.9-1) taking into account heterogeneity effect.

If IC3=1 (Sect.2.2) is specified, the nuclide dependent Dancoff correction factor internally calculated by the collision probability method is used in the heterogeneous term.

= 3 Effective only PEACO routine is used and if this nuclide is a constituent of non-resonant material. The tabulation of collision probabilities (P_{ij}) will be made by each fine-group (Users group structure) considering the change of cross-section of this nuclide by group.

= 4 Effective only PEACO routine is used and if this nuclide is a constituent of non-resonant material. Two-dimensional P_{ij} tabulation will be made assuming the behavior of cross-section of this nuclide as $1/\upsilon$.

<<Treatment when IRES=0 or IRES=2 is specified>>

Usually, enter IRES=2 for the heavy nuclide in fuel of which cross-sections have sharp resonance structure, otherwise IRES=0. For the nuclides born during burn-up calculation, the IRES values are given in the burn-up chain library (cf. Sect.3.3).

When PEACO routine is used, the IRES value given in MCROSS library is applied even if any value is entered for IRES. However, the input IRES is still effective in the evaluation of the self-shielding factor based on the NR approximation (applied out of the energy range of PEACO calculation).

<<Treatment when IRES=3 or IRES=4 is specified>>

In the tabulation of P_{ij} for PEACO calculation, the cross-sections of non-resonant nuclides are assumed as constant by using the value of the highest energy group of PEACO calculation, unless IRES=3 or IRES=4 is specified.

For the systems involving coolant water with boron or control rod, the specification of IRES=3 or IRES=4 for B-10 gives more exact treatment. However, treatment by IRES=3 requires the P_{ij} tabulation by energy group and that by IRES=4 does two-dimensional tabulation. Both treatments need much computer time.

3 IXMICR Indicator to write the effective cross-sections into the effective microscopic cross-section file (MICREF)

= 0 No edit.

= 1 Write the effective microscopic cross-sections into the MICREF file.

= 2 Write the microscopic cross-sections of hyperfine group structure averaged in the cell into UMCROSS file after PEACO calculation. The seventh and eighth characters of the member name are taken from the last half of CASENAME. During the cell burn-up calculation, the seventh character is overridden by *b*-tag. This option may be utilized for the output of former step in the treatment of double heterogeneity.

= 3 both of functions of IXMICR=1 & =2.

Note:

If the cell burn-up routine is used (IC20=1), the same option is available in Sect. 2.11 for the nuclides not appearing in this input section (e.g. MA or F.P.)

The effective cross-sections of hyperfine group structure written into UMCROSS file can be used in the latter step of double heterogeneity calculation by specifying the member name by IDENT with IRES=2.

4 DN Nuclide density (10^{24} n/cm^3)

In the double heterogeneity problem, enter the nuclide density averaged in the microscopic cell to the nuclide to which the microscopic cross-sections of hyperfine group structure are written in UMCROSS.

Block-3' Required if NISO>0 and DC<0 NISO*/A8, 2, 2/

1 IDENT the same as in Block-3

2 IRES the same as in Block-3

3 IXMICR the same as in Block-3

4 DN the same as in Block-3

5 DCN the Dancoff correction factor of this nuclide. Effective if IC3=0 in Block-3 of Sect.2.2.

Repeat Block-3 or Block-3' NISO times.

Repeat Block-2 through Block-3 or Block-3' NMAT times.

An example of material specifications to the system of UO_2 fuel, Zircaloy-2 cladding and coolant water is shown below, where the Dancoff correction factor is null as internally calculated by specifying IC3=1.

```
---------+---------+---------+---------+---------+--------
3   / NMAT
FUELXX1X  0 3  849.12 0.82 0.0    / 1 :UO2 FUEL
XU050001  2 0  1.05692E-03    / 1
XU080001  2 0  2.21466E-02    / 2
XO060001  0 0  4.64071E-02    / 3
CLADXX2X  0 3  586.88 0.13 0.0    / 2 : CLADDING
XZRN0001  0 0  3.80326E-02    / 1
XCRN0001  0 0  6.71520E-05    / 2
XFEN0001  0 0  1.31290E-04    / 3
MODEXX3X  0 2  578.15 0.0  0.0     / 3 : WATER MODERATOR
XH01H001  0 0  4.78704E-02    / 1
XO060001  0 0  2.39352E-02    / 2
---------+---------+---------+---------+---------+--------
```

2.10 Reaction Rate Calculation

The input of this section is optionally required if IC18=1 (Sect.2.2) is specified for the reaction rate calculation.

A common edit can be executed after any component routine for flux distribution (PIJ, ANISN, TWOTRAN, TUD or CITATION). The edit routine REACT permits the calculation of reaction (capture, fission) rate distribution of the detector with or without the filter.

(a) The reaction rate ($cm^{-3}sec^{-1}$) of the detector without filter is calculated as follows:

$$R(\vec{r}) = \sum_{g=1}^{IGMAX} \Sigma_{x,g} \Phi_g(\vec{r}) \tag{2.10-1}$$

where *IGMAX* is number of energy group, and *x* means reaction type (e.g. capture, fission, etc.).

(b) The reaction rate ($cm^{-3}s^{-1}$) of the detector with filter:

$$R(\vec{r}) = \sum_{g=1}^{IGMAX} f_g \Sigma_{x,g} \Phi_g(\vec{r}) \text{ , where } f_g \text{ is filter transmission factor} \tag{2.10-2}$$

By adjusting f_g , the integration range can be modified. The reaction types edited by (a) and (b) are Fission, Capture and Absorption (*A*=*F*+*C*).

(c) Spectrum index

As shown in the following equations (2.10-3) through (2.10-8), the fission reaction rate (*F*), capture rate (*C*) of nuclide μ in epi-thermal range (*epi*), thermal energy range (*th*) and whole energy range (*all*) are calculated as:

$$F_{epi}^{\mu} = \int_{E_{Cd}}^{\infty} N^{\mu} \sigma_f^{\mu}(E) \varphi(E) dE \text{ ,} \tag{2.10-3}$$

$$F_{th}^{\mu} = \int_{0}^{E_{Cd}} N^{\mu} \sigma_f^{\mu}(E) \varphi(E) dE \text{ ,} \tag{2.10-4}$$

$$F_{all}^{\mu} = F_{th}^{\mu} + F_{epi}^{\mu} \text{ ,} \tag{2.10-5}$$

$$C_{epi}^{\mu} = \int_{E_{Cd}}^{\infty} N^{\mu} \sigma_c^{\mu}(E) \varphi(E) dE \text{ ,} \tag{2.10-6}$$

$$C_{th}^{\mu} = \int_{0}^{E_{Cd}} N^{\mu} \sigma_c^{\mu}(E) \varphi(E) dE \text{ ,} \tag{2.10-7}$$

$$C_{all}^{\mu} = C_{th}^{\mu} + C_{epi}^{\mu}, \tag{2.10-8}$$

where E_{Cd} denotes cadmium cut-off energy that can be changed by setting the group dependent filter transmission by the user.

One pair of entries permits reaction rates of two nuclides. The spectrum indices are obtained as $\rho^{28} = C_{epi}^{28} / C_{th}^{28}$, $\delta^{25} = F_{epi}^{25} / F_{all}^{25}$, $\delta^{28} = F_{all}^{28} / F_{all}^{25}$, $C^{*} = C_{all}^{28} / F_{all}^{25}$.

Equations (2.10-3) through (2.10-8) are calculated by the code with considering spatial dependence and heterogeneity effect as:

$$R_{epi}^{\mu}(\vec{r}) = \sum_{g=1}^{IGMAX} f_g N_m^{\mu} \sigma_{m,g}^{\mu} \frac{\varphi_{m,g}}{\varphi_{x,g}} \Phi_g(\vec{r}), \quad (R=F \text{ or } C) \tag{2.10-9}$$

$$R_{epi}^{\mu}(\vec{r}) = \sum_{g=1}^{IGMAX} (1-f_g) N_m^{\mu} \sigma_{m,g}^{\mu} \frac{\varphi_{m,g}}{\varphi_{x,g}} \Phi_g(\vec{r}), \quad (R=F \text{ or } C) \tag{2.10-10}$$

where, $\sigma_{m,g}^{\mu}$ denotes the effective microscopic cross-section of the nuclide μ involved in the material m of the energy group g, $\varphi_{m,g}$ the local flux of the R-Region composed of the material m, $\varphi_{x,g}$ the average flux of x-th X-Region in the cell calculation, $\Phi_g(\vec{r})$ the flux at $\vec{r}$ obtained by a core calculation with homogenized cross-sections. The ratio $\varphi_{m.g} / \varphi_{x,g}$ represents the heterogeneity correction of local flux (disadvantage factor).

(d) Ratio of volume integrated reaction rates (only in CITATION)

$$\overline{R} = \int \sum_{g} \Sigma_{x2,g} \Phi_g(\vec{r}) dV \Big/ \int \sum_{g} \Sigma_{x1,g} \Phi_g(\vec{r}) dV, \tag{2.10-11}$$

where $\Sigma_{x1,g}$ and $\Sigma_{x2,g}$ are macroscopic cross-sections of the material specified by the user. The reaction denoted by $x1$ and $x2$ are specified among Fission, Capture, Absorption and Production. The option to change the numerator or denominator of Eq.(2.10-11) to be unity (1.0) is also prepared. The range of volume integration can be adjusted by input. This volume integration option is applicable only for the flux calculated by CITATION.

The cross-sections for the detectors have to be prepared before entering this routine (macroscopic ones in MACRO or MACROWRK for (a), (b) and (d) reaction rate ratio, and microscopic ones in MICREF for (c) spectrum index).

Following input data are required if IC18 > 0 in Sect.2.2.

Block-1 Control integers for reaction rate calculation /4/

1 IOPT(1) Number of detectors used without filter.
(number of repetition of reaction rate calculations)

2 IOPT(2) Number of detectors used with filter.

3 IOPT(3) Number of cases to calculate the spectrum index.

4 IOPT(4) Number of cases to calculate volume integrated reaction rate ratio (by CITATION)

Block-2-1 Control for detectors without filter, required if IOPT(1)>0. /A8, 2, 0/

1 MTNAME Member name of the detector cross-sections by 8 characters

2 IREAC Specification of reaction type
= 0 fission ($\Sigma_{x,g} = \Sigma_{f,g}$)
= 1 capture ($\Sigma_{x,g} = \Sigma_{c,g}$)
= 2 absorption (fission + capture)

3 NMESH Number of spatial points (mesh intervals) to calculate the reaction rates

Block-2-2 Required if IOPT(1)>0 /3*NMESH/

((MESH(*i*,*n*), *i*=1,3), *n*=1,NMESH)

Spatial position by mesh number, where *i*=1 corresponds to X-direction, *i*=2 to Y-direction and *i*=3 to Z-direction. In one- or two-dimensional case, enter zero values into irrelevant data. If the output of the PIJ is processed, specify R-Region number as if one-dimensional calculation.

Repeat Block-2-1 through Block-2-2 IOPT(1) times.

Block-3-1 Control for detectors with filter, required if IOPT(2)>0 /A8, 2, 0/

1 MTNAME Material name of the detector cross-sections by 8 characters

2 IREAC Specification of reaction type

= 0 fission ($\Sigma_{x,g} = \Sigma_{f,g}$)

= 1 capture ($\Sigma_{x,g} = \Sigma_{c,g}$)

= 2 absorption (fission + capture)

3 NMESH Number of spatial points (mesh intervals) to calculate the reaction rates

Block-3-2 Required if IOPT(2)>0 /3*NMESH/
((MESH(*i*,*n*),*i*=1,3), *n*=1,NMESH)

Spatial position by mesh number, where *i*=1 corresponds to X-direction, *i*=2 to Y-direction and *i*=3 to Z-direction. In one- or two-dimensional case, enter zero values into irrelevant data. If the output of the PIJ is processed, specify R-Region number as if one-dimensional calculation.

Block-3-3 Required if IOPT(2)>0 /IGMAX/
(FG(*g*),*g*=1,IGMAX)

Transmission (used in Eq.(2.10-2)) has to range between 0.0 and 1.0.

IGMAX is number of energy groups (IGMAX=NEF+NET for fine group calculation and IGMAX=NERF+NERT for few group one, cf. Sect.2.2)

Note:

If the exact values are required around the cut-off energy, print out the collision probabilities calculated in an isolated cell composed of a detector covered by a filter. The probability P_{is} is the probability that a neutron born in region i escapes from the outer surface of the filter. Then, calculate G_i by $G_i = 4V_i/S^*\Sigma_i P_{is}$ where $G_i = G_d$ (i is detector region) the probability that a neutron impinging into filtered detector from the outer surface with isotropic angular distribution.

Repeat Block-3.1 through Block 3-3 IOPT(2) times.

Block-4-1 Input for spectrum index, required if IOPT(3)>0 /6, IGMAX/

1 MPOS Material number in which the nuclides for spectrum index calculation are involved. Material number is the order of appearance in the material specification in Sect.2.9.

2 U235 The position of the first nuclide in the material. Count the position in the order of material specification.

3 U238 The position of the second nuclide in the same material. Count the position in the order of material specification.

4 IX Mesh number of X-direction where the neutron spectrum is obtained. Enter R-Region number for the collision probability calculation as it can be assumed as one-dimensional calculation.

5 IY Mesh number of Y-direction where the neutron spectrum is obtained.
Enter IY=0 for one-dimensional calculation.

6 IZ Mesh number of Z-direction where the neutron spectrum is obtained. Enter IZ=0 for one- and two-dimensional calculations.

(FGS (g),g=1,IGMAX)

Filter transmission by energy group(g), where $0 \le f_g \le 1$. They are applied in Eqs.(2.10-9) and (2.10-10). IGMAX is number of energy groups (IGMAX=NEF+NET for fine group calculation and IGMAX=NERF+NERT for few group one, cf. Sect.2.2)

Repeat Block-4-1 IOPT(3) times.

Block-5-1 Required if IOPT(4)>0 and after CITATION calculation /1/

NZONE Number of zones used in CITATION calculation (=NM of Block-1 in Sect.2.8)

Block-5-2 Required if IOPT(4)>0 and after CITATION calculation /A8/

MTNAME(i) Material name of the detector assigned to zone i.

The member of this name must be prepared on MACRO or MACROWRK file. The fifth character (e-tag) and the eighth one (p-tag) may be arbitrary as they are specified by the code (cf. Sect.2.9).

If a blank material name is entered, the corresponding zone is excluded from the integration.

Repeat Block-5-2 NZONE times.

Block-5-3 Required if IOPT(4)>0 and after CITATION calculation /2/

1 IREAC1 Reaction type for the numerator of Eq.(2.10-11)

= -1 fix as unity (=1.0)

= 0 fission reaction ($\Sigma_{x1,g}=\Sigma_{f,g}$)

= 1 capture reaction ($\Sigma_{x1,g}=\Sigma_{c,g}$)

= 2 absorption reaction ($\Sigma_{x1,g}=\Sigma_{a,g}$)

= 3 neutron production reaction ($\Sigma_{x1,g}=\nu\Sigma_{f,g}$)

2 IREAC2 reaction type of the denominator of Eq.(2.10.11)

= -1 fix as unity (=1.0)

= 0 fission reaction ($\Sigma_{x2,g}=\Sigma_{f,g}$)

= 1 capture reaction ($\Sigma_{x2,g}=\Sigma_{c,g}$)

= 2 absorption reaction ($\Sigma_{x2,g}=\Sigma_{a,g}$)

= 3 neutron production reaction ($\Sigma_{x2,g}=\nu\Sigma_{f,g}$)

Repeat Block-5-3 IOPT(4) times.

An example to use reaction rate calculation option is shown below. A pin rod cell is calculated by PIJ with 107 group (fast 62, thermal 45 groups) structure where fuel region is sub-divide into 5 R-Regions. Spatial distributions of absorption rate in the whole energy range and thermal fission rate, and spectrum indexes about U-235 and U-238 will be edited.

```
---------+---------+---------+---------+---------+--------
3   / NMAT
FUELXX1X 0 3 849.12 0.82 0.0 / l:U02 FUEL
XU050001 2 0 1.05692E-03 / l
XU080001 2 0 2.21466E-02 / 2
X0060001 0 0 4.64071E-02 / 3
CLADXX2X 0 3 586.88 0.13 0.0 / 2:CLADDING
XZRN0001 0 0 3.80326E-02 / l
XCRN0001 0 0 6.71520E-05 / 2
XFEN0001 0 0 1.31290E-04 / 3
MODEXX3X 0 2 578.15 0.00 0.0 / 3 :WATER MODERATOR
XH01H001 0 0 4.78704E-02 / l
X0060001 0 0 2.39352E-02 / 2
& << input for reaction rate calculation option >>
l l 5 0 / Block-l
FUELX01X 2 5 / Block-2-1 (total absorption rate distribution)
l 0 0  2 0 0  3 0 0  4 0 0  5 0 0 / Block-2-2
FUELX01X 0 5 / Block-3-1 (thermal fission rate distribution)
l 0 0  2 0 0  3 0 0  4 0 0  5 0 0 / Block-3-2
62(0.0) 45(1.0) / Block-3-3 filter for 62+45=107groups
l 1 2 1 0 0 62(1.0) 45(0.0) / Block-4-1 for spectral index
l 1 2 2 0 0 62(1.0) 45(0.0) / repeat Block-4-1 IOPT(3) times
l 1 2 3 0 0 62(1.0) 45(0.0)
l 1 2 4 0 0 62(1.0) 45(0.0)
l 1 2 5 0 0 62(1.0) 45(0.0)
---------+---------+---------+---------+---------+--------
```

2.11 Cell Burn-up Calculation

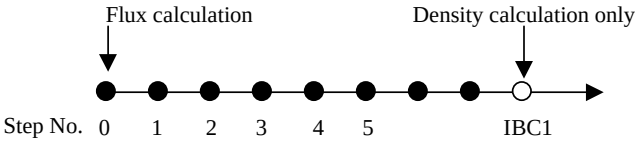
The input of this section is required if IC20=1 (Sect.2.2) is specified for cell burn-up calculation. The information such as burn-up chain scheme, yield, decay constant, power per fission, etc. is read from the logical unit 50. Several files are prepared for the optional use of burn-up chain models. As these files are written by text format, the user can easily modify or compile his own file. The contents and structure are described in Section 3.3.

Block-1 Control integers for optional use /20/

IBC1 Final burn-up step number (<MXSTEP)

The value of IBC1 is the same as number of burn-up steps, unless it is for restart burn-up calculation activated by negative IBC3 below. The MXSTEP(=61) is the upper limit defined by code. In the restart calculation, IBC1 must be larger than the step number that the previous calculation stopped at.

A burn-up step number for edits starts from zero, which corresponds to fresh fuel condition. At each burn-up step point, flux calculation is carried out and results are printed and stored in PDS files. At the last step point (step number=IBC1), flux calculation is skipped although fuel composition is calculated. If results like k_{eff} at the last step point, a dummy step point is required at the last.



The 6-th character (cf. *b*-tag in Sect.2.9) of the name of each member in PDS files is named as follows:

0, 1, 2, 3,….., 9, A, B, C,…., Z, a, b, c,……z

IBC2 Unit of burn-up for the entries of Block-3

= ±1 Integrated burn-up by MWd/t (MWday per 10^3kg of initial heavy metals)

= ±2 Integrated burn-up by MWd

= ±3 Integrated burn-up by day

= ±4 Burn-up interval of each step by day

= ±5 Depletion fraction of U-235 atomic number density to the fresh one by percent (0.0~100.0)

Note:

If negative number is entered for IBC2, the nuclide for depletion fraction in output edit is replaced from U-235 by that specified by Block-4. Especially for IBC2=-5, the burn-up step is defined by depletion fraction of the specified nuclide.

IBC3 Burn-up mode

= ±1 Normal burn-up calculation

= ±2 Branch-off calculation (entry Block-5 is required)

= ±3 Burn-up calculation under constant flux

= ±4 Burn-up calculation by reading initial composition from Block-6

Note:

If negative number is entered for IBC3, restart calculation is executed to succeed the last step of the previous calculation of the same case name.

The following burn-up calculation modes can be selected here.

- Normal burn-up calculation: The depletion equation is solved by assuming constant power level in each burn-up step interval. (cf. Sect.7.7)
- Branch-off calculation: Depletion equation is not solved. After the normal burn-up calculation, cell calculation is performed along burn-up by using the fuel composition obtained by the normal burn-up mode but in the different cell conditions (e.g. temperature, void fraction, boron concentration, etc.)
- Constant flux calculation: In the blanket fuel, power density increases in proportion to production of fissile nuclides. In such a case, the normal burn-up calculation model may be not proper. In this mode, a burn-up calculation is performed with constant flux level determined by the initial power or input value. In the latter case, burn-up calculation is possible for the cell including burnable nuclides but no fissionable ones.
- Burn-up by reading initial composition: After a normal burn-up calculation, new case of burn-up calculation can be done in different cell conditions by reading the fuel composition from the normal calculation result at an arbitrary burn-up step.

IBC4 Edit option

= 0 Brief edit (for usual case, summary is printed on 98th device)

= 1 Detailed edit (one group microscopic cross-sections is printed on 99th device)

= 2 Information for debugging

= 3 Detailed information for debugging

IBC5 Definition of instantaneous conversion ratio

= 0 Use defaulted definition of conversion ratio

= 1 Conversion ratio is redefined by entries of Block-7-1 through -7-3

Note:

Generally, an instantaneous conversion ratio is defined as the ratio of production rate to depletion rate of fissile nuclides as follows:

$$\text{Instantaneous CR}(t) = \frac{\text{FISSProduction}(t)}{\text{FISSDepletion}(t)}. \tag{2.11-1}$$

In the SRAC, the user can flexibly define the numerator and denominator of Eq.(2.11-1). They are calculated by Eqs.(2.11-2) and (2.11-3), respectively. (Both are the same function forms)

$$\text{FISSP}(t) = \int \left[\sum_{g} \sum_{i \in Specified} \left\{ \alpha^i < N^i(t) > \sigma^i_{x(i),g}(t)\, \Phi_g(t) + \beta^i \lambda^i N^i \right\} \right] dV \tag{2.11-2}$$

$$\text{FISSD}(t) = \int \left[\sum_{g} \sum_{j \in Specified} \left\{ \alpha^j < N^j(t) > \sigma^j_{x(j),g}(t)\, \Phi_g(t) + \beta^j \lambda^j N^j \right\} \right] dV \tag{2.11-3}$$

where,

i , j	:	any nuclides selected from the burn-up chain library used,
α , β	:	arbitrary factors defined by user, which are used to consider branching ratio or to cut of unnecessary terms (e.g. β = 0.0),
$< N^i >$	:	atomic number density of nuclide i or 1.0 to define microscopic reaction rate,
$\sigma^i_{x(i)}$	:	microscopic cross-section of nuclide i for reaction type x. The reaction type is determined by user depending on nuclide i,
λ	:	decay constant of each nuclide whose value is defined in the burn-up chain library. (cf. Sect.3.3)

Furthermore, integrated conversion ratio is also calculated as follows:

$$\text{Integrated CR}(t) = \frac{\int_0^t \text{FISSProduction}(\tau)d\tau}{\int_0^t \text{FISSDepletion}(\tau)d\tau}. \qquad (2.11\text{-}4)$$

Thus the user can calculate his own microscopic or macroscopic reaction rates and their ratio by the option IBC5=1.

The defaulted definition of conversion ratio follows the description in the burn-up chain library. As the initial setting, it is defined as the ratio of the summation of capture reaction rates of Th-232 (if any in chain), U-234 (if any), U-238 and Pu-240 to the summation of absorption reaction rates of U-233 (if any), U-235, Pu-239 and Pu-241. (no decay effect)

IBC6 Option to write effective microscopic cross-sections into MICREF file

= 0 No cross-sections are written unless IXMICR (Sect.2.9) is not specified to certain nuclides. This option is suggested if MICREF file is not preserved.

= 1 Write cross-sections of the nuclides specified by Block-8

= 2 Write cross-sections of the whole depleting nuclides

= 3 Write cross-sections of the whole burnable resonant nuclides

Note:

In such a case that numbers of depleting materials, burn-up steps or depleting nuclides are large as to cause shortage of core memory for virtual PDS file, keep the requirement to write cross-sections to a minimum.

[cf.] Sect.1.4, Block-5 in Sect.2.2, Block-3 in Sect.2.9

IBC7 Option to make up collision probability table for PEACO calculation (effective if IC5=±2 is specified in Sect.2.2)

= 0 Update at each burn-up step (suggested)

= 1 Make up tables at first two steps and use the second one after that

Note:

Option IBC7=1 is used to reduce large CPU time.

IBC8 Maximum length (LCHA) of decay chain in linear analysis

= 0 Defaulted value (LCHA=6) is used

> 0 Input value is used for LCHA. If large LCHA is used, as number of

chains under consideration is enlarged, long CPU time and large core memory are required.

IBC9 Option to fix atomic number densities of specified nuclides

= 0 Calculate atomic number densities of all nuclides

= *N* Replace atomic number densities of *N* nuclides by the values specified by Block-11.

Note:

This option is used, for example, to prepare Xenon free cross-sections for a branch-off calculation, or to assume on-line decontamination in the normal burn-up calculation. $N \leq 5$ must be satisfied.

IBC10 Option to specify depleting material

= 0 Any material containing at least one nuclide appearing in burn-up chains is automatically assumed as depleting material.

= 1 The user specifies depleting materials by Block-9

Some burn-up chain model assumes such a material as cladding, boric water or control rod to be depleting although the user does not want to treat as depleting. This option is used to avoid it.

Note:

Especially pay attention to boric water, because B-10 is treated as a burnable nuclide in any burn-up chain model.

IBC11 through IBC20

= 0 (not used)

Block-2 Thermal power (MWt/cm) /IBC1/

(POWERL(*i*), *i*=1,IBC1)

Thermal power (MWt) in the whole cell per unit length (1cm) at each burn-up step interval. For example, to the cell containing 4 pin rods with average linear power of 170 W/cm, enter 170*4*1.0E-6=6.60E-4 as POWERL.

To a one-dimensional plane geometry, assume unit length for two transverse directions, and enter average thermal power of the system (cell thickness)*1cm* 1cm.

The geometry model in collision probability method should be taken care. For example, as the models for IGT= 8, 9, 16 calculate the collision probabilities for a quarter of a fuel assembly, enter 1/4 of assembly power as POWERL. The model for IGT=15 calculates them for a whole assembly while it assumes 60 degree rotational symmetry. Then enter the whole assembly power.

If POWERL(*i*)=0.0 is entered, the cooling calculation (reactor stop) is executed, where only radioactive decay is considered.

If IBC3=±3 is entered, the average flux in fuel zone corresponding to the initial thermal power POWERL(1) is applied through the whole steps. The thermal power at each step POWERL(*i*) after the initial step is calculated by the code regardless of input values.

Block-3 /IBC1/

(PERIOD(*i*),*i*=1,IBC1)

Burn-up period (exposure) by step in unit specified by IBC2

If cooling calculation is intended and if burn-up unit is not day (IBC2=±1, ±2, ±5), enter cooling period (day) by negative value for the step of POWERL(*i*)=0.

Block-4 Required if IBC2<0 /A4/

STDNUC Specify name of the nuclide to calculate burn-up fraction of the atomic number density instead of the defaulted nuclide U-235. Enter as ‘XU03’ or ‘XPU9’ (cf. Sect.8.1). Any character is accepted for the first character.

Note:

The defaulted ‘XU05’ must be changed, if U-235 is not included in the fresh fuel, to avoid zero division.

Block-5 Required if IBC3=±2 /A4/

CASBRN Enter case name by 4 characters to refer in the branch-off calculation.

In the branch-off calculation a series of cell calculations are executed without depletion calculation by reading the composition of each burn-up step from the existing member; ‘CASBRN’BNUP on MACRO or MACROWRK file.

[cf.] Sect.3.1

Block-6 Required if IBC3=±4 /A4, 1, 0/

1 CASINT Enter case name by 4 characters to read the initial composition. The composition at each burn-up step is stored in the existing member; ‘CASINT’BNUP on MACRO or

MACROWRK file.

2 INTSTP Step number to read the composition. Enter 0 if the burn-up step tag (*b*-tag) is '0'. The *b*-tags (cf. Sect.2.9) correspond to burn-up step numbers as:
(*b*-tag=0, 1,…,9, A, B,…,Z, a, b,….,z ⇒ 0, 1,….,9, 10, 11, …35, 36, 37,....,61)

Block-7-1 Required if IBC5=1 /2/

1 NFIS Number of nuclides to contribute to depletion of fissile nuclides
See Eq.(2.11-3) and burn-up chain model (cf. Sect.3.3)

2 NFER Number of nuclides to contribute to production of fissile nuclides
See Eq.(2.11-2) and burn-up chain model (cf. Sect.3.3)

Block-7-2 Required if IBC5=1 /A4, 1, 1/

1 NAMFIS Nuclide name and reaction type to contribute to depletion of fissile nuclides by 4 characters. The first 3 characters are for nuclide name and the fourth character for reaction type (Fission/ Capture/ Absorption/ N2N/ Decay). Enter as 'U05A', 'U08C', 'PU1D'. If 'D' is specified, contribution of decay is included in the calculation of conversion ratio whereas this contribution is not taken into account for the tabulated absorption cross-section of fissile material ($\Sigma_{a,g}^{fissile}$) to be stored in MACRO file.

Note:

Nuclide name and reaction type should be appropriately selected by taking into account the burn-up chain model used in the calculation. (cf. Sect.3.3)

The fissile absorption cross-section ($\Sigma_{a,g}^{fissile}$) is used by COREBN to calculate conversion ratio.

2 IFISFLG

= 0 Do not multiply atomic number density of this nuclide (microscopic cross-sections are used)

= 1 Multiply atomic number density of this nuclide (macroscopic cross-sections are used)

3 FISFACT The factor to indicate sign or branching ratio. If Block-7-2 are entered as below, the summation of the values in parentheses is defined as the depletion rate of fissile

material (denominator of conversion ratio calculation: Eq.(2.11-3))

U03A	1	+1.0	$(+N^{\text{U-233}}\sigma_a^{\text{U-233}}\Phi)$
U05A	0	+0.5	$(+0.5\times\sigma_a^{\text{U-235}}\Phi)$
PA3A	1	-1.0	$(-N^{\text{Pa-233}}\sigma_a^{\text{Pa-233}}\Phi)$
PU1D	1	+0.2	$(+0.2\times\lambda^{\text{Pu-241}}N^{\text{Pu-241}})$

However, the tabulated values of fissile absorption cross-sections along burn-up are defined as:

$\Sigma_a^{fissile} = N^{\text{U-233}}\sigma_a^{\text{U-233}} + 0.5*\sigma_a^{\text{U-235}}\Phi - N^{\text{Pa-233}}\sigma_a^{\text{Pa-233}}$,

where no contribution of decay is included.

Repeat Block-7-2 NFIS times.

Block-7-3 Required if IBC5=5 /A4, 1, 1/

1 NAMFRT Number of nuclides to contribute to production of fissile nuclides by 4 characters. The first 3 characters are for nuclide name and the fourth character for reaction type (Fission/ Capture/ Absorption/ N2N/ Decay). Enter as; ‘U08C’, ‘PU0C’, ‘PU0N’.

Note:

Nuclide name and reaction type should be appropriately selected by taking into account the burn-up chain model used in the calculation. (cf. Sect.3.3)

Even if ‘D’ is specified, contribution of decay is not reflected in the tabulation of capture cross-section of fertile material ($\Sigma_{c,g}^{fertile}$) to be stored in MACRO file. The fertile capture cross-section ($\Sigma_{c,g}^{fertile}$) is used by COREBN to calculate conversion ratio together with fissile absorption cross-section ($\Sigma_{a,g}^{fissile}$).

2 IFRTFLG

= 0 Do not multiply atomic number density of this nuclide (microscopic cross- sections are used)

= 1 Multiply atomic number density of this nuclide (macroscopic cross-sections are used)

3 FRTFACT The factor to indicate sign or branching ratio. (same as FISFACT in Block 7-2)

Repeat Block-7-3 NFER times.

Block-8-1 Required if IBC6=1 /1/

NMICR Number of nuclides of which effective cross-sections are written on MICREF file

Block-8-2 Required if IBC6=1 /NMICR/, (18A4)

NAMMIC Names of nuclides of which effective cross-sections are written on MICREF file. Enter by 3 characters and one arbitrary character. The microscopic cross-sections of the specified nuclide are written for every material in which the nuclide is contained.

Sample input: U08_B00_PU9_ (the fourth character is ineffective)

Block-9 Required if IBC10=1 /NMAT/

(IBTYPE(*i*), *i*=1,NMAT)

= 0 Non-depleting material

= 1 Depleting material

Enter IBTYPE(*i*) to material *i* to specify if it is depleting or not. NMAT is number of materials, and material is numbered in the order appearing in the material specifications. (cf. Sect.2.9). Specify IBTYPE(*i*)=0 to a material composed of the nuclides which do not appear in the selected burn-up chain model.

Block-10 Required if IBC3=±3 and no fissionable nuclide is contained in any material /1/

FLXLVL When the system does not contain any fissionable nuclide but depleting nuclide like burnable poison, depletion calculation is available under fixed flux condition by specifying IBC3=±3. Enter average flux level (n/cm^2/s) to the burnable region. Unit of burn-up (MWd/t, MWd) is replaced by the integrated absorption reaction rate. The use of this option requires to specify IBC2=±3 or =±4.

Block-11-1 Required if IBC9>0 /A4/

NAMFP Name of nuclide of which number densities are specified by input values.

Sample: XE5_ (the first 3 characters are effective)

Block-11-2-1 Required if IBC9>0 /1/

MPOS = 0 End of Block-11-2 entries

> 0 Material number for which the atomic number density of the nuclide is replaced. Material is numbered in the order appearing in the material specification (Sect.2.9).

Block-11-2-2 Required if IBC9>0 and MPOS>0 /IBC1+1/

DENFP Atomic number density (*10^{24} n/cm^3) at every burn-up step (0,1, 2,…,IBC1)

Repeat Block-11-2 until MPOS=0 is encountered.
Then repeat Block-11-1 through Block-11-2 IBC9 times.

<<Sample input of Block-11 for IBC9=2>>

```
XE5          / NAMFP (Block-11-1)
1            / MPOS(Block-11-2-1) for 1st Fuel
11(0.0)            / DENFP (Block-11-2-2)
5            / MPOS for 2nd Fuel
11(0.0)            / DENFP
0            / MPOS=0 : End for Xe-135
SM9          / NAMFP (Block-11-1)
1            / MPOS(Block-11-2-1) for 1st Fuel
11(1.23E-4 )       / DENFP (Block-11-2-2)
5            / MPOS for 2nd Fuel
11(1.23E-4) / DENFP : Peak Sm-149
0            / MPOS=0 : End for Sm-149
```

The following notices and recommendations would be helpful for the use of burn-up calculation.

- Burn-up step interval

At every burn-up step, effective microscopic cross-sections and flux distribution are updated and output edit is prepared. As change of composition is calculated by an analytical method at every sub-step (10 sub-steps in the initial step to accurately consider Xenon buildup and 3 sub-steps after that are internally set), the interval has not necessarily to be short. Normally, 5,000 ~ 10,000 MWd/t is used. However, the initial Xenon buildup and the treatment of burnable poison of relatively short lifetime should be taken care of.

- Multiplication factor and cross-sections at the final step

At the end of final burn-up step, the composition of depleting material is edited, but the spectrum calculation for this composition is not executed. Therefore, values are not printed out for multiplication factor and conversion ratio corresponding to the final composition. Neither cross-sections nor flux are written into PDS files.

The user should keep in mind that the step before the last gives the upper limit of burn-up in the tabulation of cross-sections for the succeeding use of COREBN.

- Chemical binding effect of fuel material

Mixed use of U08W (chemical binding of UO_2 is reflected) and U080 (free gas model) should

be avoided. Because U08W and U080 are not discriminated in the depletion calculation, use of only U080 is recommended. It is to be noted that there is no significant effect by chemical binding of UO_2 in usual thermal reactor calculations.

- Plural X-Region specification

When plural X-Regions are specified, one depleting material should not be contained in two different X-Regions.

- Restart burn-up calculation

The restart burn-up calculation is available as far as members *case*HT*jj* (cf. Sect.3.1) of the same case name are preserved on MACRO or MACRWRK (no collapsing is done) file. The change of input data is limited, in principle, only on restart specification and addition of burn-up steps.

Even in the case of abnormal termination due to lack of CPU time or shortage of disk extent, if the members *case*HT*jj* are preserved on MACRO or MACRWRK file, the calculation can be continued by using this restart option. However, if the virtual PDS file is used, the members are not stored in the case of some abnormal terminations. To avoid such a trouble in a large-scale burn-up calculation, it is recommended to set IOMODE (access mode of MACRO file) to 'File' (direct file access) in Block-5 of Sect.2.2.

- Branch-off calculation

The branch-off calculation along the burn-up steps is available if the member *case*BNUP of the reference case is preserved on MACRO or MACROWRK (no collapsing is done) file. The input for geometry, number of burn-up steps, burn-up intervals, etc. must be consistent with those of the reference case. Number of materials, the order of materials (=material number) and the burn-up chain model must be also kept in principle, whereas material temperatures, composition of non-depleting materials may be replaced.

For example, when the average cross-sections of the assembly with control rod insertion is obtained by the branch-off calculation, the region in which the control rod is inserted should be reserved as an R-Region in the reference calculation without control rod insertion.

If the control rod material contains any nuclide which appears in the burn-up chain model, the material should be specified as non-depleting by using the option IBC10=1.

As coolant water of PWR containing boron circulates in primary circuit, this material should be treated as non-depleting. The reference burn-up calculation may treat the condition without boron, and the branch-off calculation treat the condition with boron. In the latter condition, the coolant containing

boron should be specified as non-depleting to keep the number of depleting materials.

- Burn-up calculation by reading the initial composition

To execute the burn-up calculation by reading the initial composition, the member *case*BNUP (cf. Sect.3.1) of the reference case must be preserved on MACRO or MACROWRK file. Input data for geometry, number of materials, the order of materials (=material number), the burn-up chain model, etc. used in the reference case must be consistent in the calculation.

- Cooling calculation

The cooling calculation, mainly, aims to study the effect of decay of short lived nuclides after reactor shut down. When this cooling option is used to evaluate radio-toxicity during several thousands of years, the decay chain models formed to study burn-up behavior in reactors should be carefully checked. Some model, for example, skips production paths because of the long half-life compared with neutron absorption reaction.

2.12 PEACO ; The hyperfine Group Resonance Absorption Calculation

The input of this section is required when PEACO routine is used for effective microscopic resonance cross-sections by specifying IC5=2 or -2 (Sect.2.2).

Block-1 /1/

IPLOT Plot control for spectra by PEACO in resonance energy range

Plot data is stored as a PostScript file (cf. Sect.1.11).

= 0 Skip plot

= ±1 Plot neutron spectra by up-to five R-Regions in one figure

= ±2 Plot neutron spectra by R-Region for an R-Region per figure

= ±3 Plot neutron spectra by up-to five R-Regions in one figure in the energy ranges which are specified in Block-3 and -4.

Note:

If negative value is entered, group cross-sections modified by PEACO calculation are printed out in the users fine-group structure.

Block-2 Required if IC5=-2 /NMAT/

(IRX(*i*),*i*=1,NMAT)

PEACO routine has a restriction so that one or two independent resonant material(s) can be treated, where an resonant material is defined as a material to contain at least one nuclide of which cross-sections are stored in MCROSS file. When more than two resonant materials exist in the system, they must be classified into one of two groups by their characteristics. This item specifies the material group in the order appearing in the material specifications (Sect.2.9)

= 0 Non-resonant region

= 1 Assign to the first resonant material

= 2 Assign to the second resonant material

Note:

PEACO routine calculates the collision probabilities by interpolation of tabulated probabilities by using the total cross-section as argument. Such tabulation can be prepared for the combination of two different total cross-sections. This is the reason of the restriction. If the third resonance material has almost same energy structure with any of two materials, an approximation to assume the third is equivalent to any of the two holds. Most of resonance absorption is, as known,

contributed by U-238. When the resonance materials are mainly composed by U-238, the extension to permit more than two resonant materials can be applied. For example, it can be applied to the burn-up calculation of multilayer pin cell model. Each layer initially of uniform composition will have gradually different Pu content along burn-up. Each can be classified into inner fuel region or outer fuel region where Pu content is higher in outer region.

Block-3 Required if IPLOT=3 /4/

(EL(*i*),*i*=1,4) The lower energy boundaries of 4 energy ranges for plotting the spectra. In the first figure, spectra are plotted in the first energy range from EL(1) to EH(1).

Block-4 Required if IPLOT=3 /4/

(EH(*i*),*i*=1,4) The upper energy boundaries of 4 energy ranges for plotting the spectra.

3. I/O FILES

We shall describe the structure of I/O files and their physical contents that will be helpful to prepare the input and to utilize the output.

The I/O files used in SRAC are divided into PDS files (described in Sect.1.4) and sequential data set files (PS files). Their contents will be described in this chapter.

3.1 Contents of PDS files

Ten PDS files below are used. The strings appearing in [ ] are the file name used in this document.

- Public Fast Library [PFAST]
- Public Thermal Library [PTHERMAL]
- Public MCROSS Library [PMCROSS]
- User Fast Library [UFAST]
- User Thermal Library [UTHERMAL]
- User MCROSS Library [UMCROSS]
- Fine Group Effective Microscopic Cross Section File[MICREF]
- Fine Group Macroscopic Cross Section File [MACROWRK]
- Coarse (Few) Group Macroscopic Cross Section File [MACRO]
- Flux File [FLUX]

The contents of each file will be described separately. Several pairs of files appear in the above list: Public Fast and User Fast files, Public Thermal and User Thermal files, and Public MCROSS and User MCROSS files. The structure of User file and Public one is common except MCROSS file: Public MCROSS file contains point-wise cross-sections and User MCROSS file contains Doppler broadened hyperfine group cross-sections. While the Public files contains the data of every possible nuclides, the User one keeps the data of the nuclides specified by the user for a series of calculations. The data in User Fast and Thermal files are collapsed into the user’s collapsed energy group structure by using the neutron spectrum installed in the Public ones. The Public files are accessed as read-only files.

Although all the members of PDS files keep the member length at the top of each member (cf. Sect.1.4), the description hereafter does not specify it.

3.1.1 Public Fast Library [PFAST] / User Fast Library [UFAST]

The microscopic fast group cross-section files [PFAST] [UFAST] keep infinitely diluted microscopic cross-sections, the tables for self-shielding factors, and resonance level parameters in the fast groups by nuclide.

The following 13 kinds of members are stored in the library.

Member name	Contents
FASTLIB	Control information for the whole library such as energy group structure, asymptotic neutron spectrum for collapsing
FISSYILD	Pseudo fission neutron yield that is used for the fixed source non-fissile material
C*zzm*0000	Control information for the nuclide *zzm* such as presence of self-shielding factor tabulation, resonance level parameters and fission cross-sections
M*zzm*0000	Infinitely diluted cross-sections for the nuclide *zzm*
F*zzm*0000	Self-shielding factor table for the nuclide *zzm*
R*zzm*0000	Control information for resonance parameters of the nuclide *zzm*
P*zzm*000*l*	Resonance parameters for *l*-state of the nuclide
B*zzm*000*r*	Background cross-sections for the reaction *r* of the nuclide *zzm*, where *r*=F (fission), *r*=C(capture), *r*=E (elastic)
Y*zzm*0000	Delayed neutron parameters for fissile nuclide
Q*zzm*0000	P_2 component of the elastic scattering
S*zzm*0000	P_3 component of the elastic scattering
T*zzm*0000	P_4 component of the elastic scattering
U*zzm*0000	P_5 component of the elastic scattering

zzm Nuclide identification composed of chemical symbol of the nuclide and the last digit of the mass number. The available combination of *zzm* is listed in Sec.8.1.

Member **FASTLIB** /2*NGF+5/

The member keeps the information about the energy group structure in a vector.

NGF Total number of energy groups.

= 74 (E_c=0.414eV) in the public library

NGF1, NGF2, NGF3

The lowest group number in each energy range of the fast (1MeV), smooth (50keV) and resonance-I (130.07eV), respectively. The NGF-th group must be the lowest in the resonance-II range. (cf. Sect.1.5)

(W(*g*),*g*=1,NGF)

Weighted lethargy widths which will be used in collapsing the energy group

structure.

(E(g),g=1,NGF+1)

Boundary energies in eV.

Member **FISSYILD** /NGF/

The member keeps the fission neutron yield of U-235 to provide the fixed source in calculating the fast neutron spectrum for non-fissile material.

(X(g),g=1,NGF)

Fission neutron yields in the g-th group normalized as

$$\sum_g \mathrm{X}(g) = 1.0$$

Member **C*zzm*0000** /42/

The member keeps the control information of the nuclide in a vector.

ICAP = 0 No capture

= 1 Capture cross-sections stored

IFISS = 0 No fission

= 1 Fission cross-sections stored

IRP = 0 No resonance parameter

= 1 Resonance parameters used in the IR approximation.

LTOT Vector length of the member M*zzm*0000 described below.

(LTH(i),i=1,4) Partial vector length which contains the i-th scattering matrix, where i=1 for inelastic, i=2 for (n,2n), i=3 for elastic P_0 and i=4 for elastic P_1.

(LA(i),i=1,4) The lowest group number of the energy range where the i-th scattering occurs.

(LD(i),i=1,4) Number of energy groups to which the slowing-down occurs in the i-th scattering.

IFS Index for shielding factor tables

= 0 No shielding factor

= 1 Shielding factors for any reaction are tabulated

IFTR, IFC, IFF, IFE, and IFER

Indices for self-shielding factor tables for partial reaction of transport, capture, fission, elastic and elastic slowing-down, respectively.

NGMIN and NGMAX

The highest and lowest group number for self-shielding factor tabulation.

NSIGF Number of admixture cross-sections which are used as one of the arguments for interpolation of self shielding factor.

NTEMPF Number of temperatures which are also used as one of the arguments for interpolation of self-shielding factor.

AMASS, SIGP, and SIGC0

Properties of the nuclide; atomic mass in amu, potential scattering cross-section and the 2200 m/sec value of capture cross-section.

(TEMP(t),t=1,4)

Temperatures (K) for the self-shielding factor tabulation. Zero value is filled for TEMP(t >NTEMPF)

(SIG0(i),i=1,8)

Admixture cross-sections for self-shielding factor tabulation. Zero value is filled for SIG0(i >NSIGF)

IPL Order of elastic scattering. (cf. Sect.8.2)

Member **Mzzm0000** /LTOT/

The member keeps the principal neutron cross-sections.

(CAPT(i),i=1,NGF)

Capture cross-sections if ICAP=1.

(FISS(i),i=1,NGF)

Fission cross-sections if IFISS=1.

(FNU(i),i=1,NGF)

ν : Neutron yield per fission if IFISS=1.

(FSPC(i),i=1,NGF)

χ : Fission neutron spectrum if IFISS=1.

(TR(i),i=1,NGF)

Transport cross-sections

(WEIGHT(i),i=1,NGF)

Lethargy widths weighted by fission neutron spectrum

(ELAS(i),i=1,NGF)

Total elastic cross-sections

(N-N(i),i=1,LTH(1))

Inelastic scattering matrix of the length

LTH(1) = (LD(1)+1)*LA(1), ordered as,

$\sigma_{1\to1}$, $\sigma_{1\to2}$,……., $\sigma_{1\to1+LD(1)}$,

$\sigma_{2\to2}$, $\sigma_{2\to3}$,……, $\sigma_{2\to2+LD(1)}$,

……

$\sigma_{g\to g}$, $\sigma_{g\to g+1}$,…, $\sigma_{g\to g+LD(1)}$,

……

(N2N(*i*),*i*=1,LTH(2))

(n,2n) scattering matrix of the length

LTH(2) = (LD(2)+1)*LA(2).

(ELP0(*i*),*i*=1,LTH(3))

Elastic P_0 scattering matrix of the length

LTH(3) = (LD(3)+1)*LA(3).

(ELP1(*i*),*i*=1,LTH(4))

Elastic P_1 scattering matrix of the length

LTH(4) = (LD(4)+1)*LA(4).

Member **Fzzm0000** if IFS=1

/NSIGF*NTEMPF*(NGMAX-NGMIN+1)*(IFTR+IFC+IFF+IFE+IFER+1)/

The member keeps the self-shielding factor table:

((FTABF(*i*,*t*,*g*,*n*),*i*=1,NSIGF),*t*=1,NTEMPF),*g*=NGMIN,NGMAX),*n*=1,NSF+1)

where, NSF=IFTR+IFC+IFF+IFE+IFER.

First, the self-shielding factors are repeated for the reaction type which has the self-shielding factor table. At the last part of the member (n=NSF+1), weighting data for energy collapsing from Public Library to User Library are stored.

Member **Rzzm0000** if IRP=1 /6/

The member keeps the control information for resonance level parameters.

NLS	Number of neutron orbital angular momentum
SPI	Nuclear spin
AP	Scattering radius in unit of 10^{-12} cm
AWR	Ratio of the mass of the nuclide to that of a neutron
EL	Lower limit for a energy range
EH	Upper limit for a energy range

Member **Pzzm0001** if IRP=1 /15*NRS+2/

The member keeps the control information for a given *l*-value, repeated for *l*=0,NLS-1.

L Value of *l*

NRS Number of resolved resonance levels for a given *l*-value.

15 resolved resonance parameters per a level to express the multi-level formula; repeated for NRS times.

ER_j Resonance energy (eV)

AJ_j Statistical factor (2J+1)/2/(I+1)

GT_j Γ : total width (eV)

GN_j Γ_n : neutron width (eV)

GG_j Γ_γ : gamma width (eV)

GF_j Γ_f : fission width (eV)

$SIGZ_j$ Peak value of total cross-section

$$\sigma_0 = 2.6 * 10^6 * (AJ_j) * \Gamma_n / (\Gamma * (ER_j))$$

$SIGZP_j$ Peak value of scattering cross-section

$$\sigma_{0p} = (\sigma_0 \sigma_p * (AJ_j) * \Gamma_n / \Gamma)^{1/2}$$

$BETA_j$ $\beta_\infty = (1.0 + (\sigma_0 \Gamma_n / \sigma_p \Gamma))^{1/2}$

ETA_j $\eta_\infty = \sigma_0 / \sigma_p$

RII_j $I_\infty = \pi \sigma_0 \Gamma_\gamma / 2ER_j$

UT_j *U*-value for total

VT_j *V*-value for total

UF_j *U*-value for fission

VF_j *V*-value for fission

for *j*=1,NRS, and σ_p is potential scattering.

Member **Bzzm000r** if IRP=1

The member keeps the background cross-sections for a given reaction

NR Number of energy ranges that have been given. A different interpolation scheme may be given for each range.

NP Total number of energy points used to specify the data.

(NBT(*i*),INT(*i*),*i*=1,NR)

Interpolation schemes

(E(*i*),σ(*i*),*i*=1,NP)

Background cross-sections

Member **Yzzm0000** if IFISS=1 /3+2*6+NGF*7/

The member keeps the information related delayed fission.

EE Incident neutron energy for the following delayed fission data in eV. (always EE= 0.0253)

NUT Total ν-value for thermal fission.

(LAMDA(j),j=1,6)

Decay constants for delayed neutron family j.

(BETA(j),j=1,6)

Fraction of delayed neutron family j. Sum of BETA(j)=1.

(NUD(g),g=1,NGF)

ν-value of delayed neutron for group g in fast energy

NUDT ν-value of delayed neutron for thermal fission

((KAID(g,j),g=1,NGF), j=1,6)

Delayed fission neutron spectrum by family j

Member **Qzzm0000** P_2 component of the elastic scattering /LTH/

(ELP2(i),i=1,LTH)

Elastic scattering matrix of the length LTH = (LD(4)+1)*LA(4).

Member **Szzm0000** P_3 component of the elastic scattering /LTH/

(ELP3(i),i=1,LTH)

Elastic scattering matrix of the length LTH = (LD(4)+1)*LA(4).

Member **Tzzm0000** P_4 component of the elastic scattering /LTH/

(ELP4(i),i=1,LTH)

Elastic scattering matrix of the length LTH = (LD(4)+1)*LA(4).

Member **Uzzm0000** P_5 component of the elastic scattering /LTH/

(ELP5(i),i=1,LTH)

Elastic scattering matrix of the length LTH = (LD(4)+1)*LA(4).

3.1.2 Public Thermal Library [PTHERMAL] / User Thermal Library [UTHERMAL]

The microscopic thermal group cross-section files [PTHERMAL], [UTHERMAL] keep the infinitely diluted microscopic cross-sections and the tables for self-shielding factors in the thermal neutron range by nuclide.

Member name	Contents
THERMAL*t*	Control information of the library
C*zzmc*000	A control member for the nuclide zzm
K*zzmc*000	Upscattering, capture, total and fission vectors and P_0 matrix (if any)
P*zzmc*000	P_1 matrix
Q*zzmc*000	P_2 matrix
S*zzmc*000	P_3 matrix
T*zzmc*000	P_4 matrix
U*zzmc*000	P_5 matrix
F*zzmc*00*r*	Shielding factor tabulation (*r*=C:captute, F:fission)
Z*zzmc*000	ν -value

zz	denotes element chemical symbol as described in Sect.8.1,
m	for last digit of mass number to discriminate isotopes (Sect.8.1),
c	for chemical compound state as shown in Sect.8.1,
t	for the temperature index (1,2,3,……..9,A,B,C) (Sect.8.1)

Member **THERMAL*t*** /2*(NGT+1)/

NGT Number of energy groups

(WT(*g*),*g*=1,NGT)

Integrated asymptotic neutron spectrum in the group which will be used as weights for collapsing the energy group structure. The spectrum is prepared to form the Maxwellian of neutron temperature (T_n=T_m+50) and 1/*E* above the cut-off of 5*kT_m, given for *g*=1,NGT.

(E(*g*),*g*=1,NGT+1)

Boundary energy of the *g*-th group in eV

Member **C*zzmc*000** /30/

INT(1) = 0 Non fissile

= 1 Fissile

INT(2)	= 0 K-member only without scattering matrix	(P_0 data without matrix)
	= 2 K- member only with P_0 matrix	(P_0 data)
	= 6 K- and P- members	(P_0 and P_1 data)
	=14 K-, P-, Q- members	(P_0-P_2 data)
	=30 K-, P-, Q-, S- members	(P_0-P_3 data)
	=62 K-, P-, Q-, S-, T- members	(P_0-P_4 data)
	=126 K-,P-,Q-,S-,T-,U- members	(P_0-P_5 data)
INT(3)	= 0 No self-shielding factor tabulation	
	= 1 Self-shielding factor tabulation	

INT(4) The highest group which has self-shielding factor (=NGMINT)

INT(5) The lowest group which has self-shielding factor (=NGMAXT)

INT(6) Number of admixture cross-sections for self-shielding factor tabulation (=NSIGT)

INT(7) Number of temperatures for which the cross-sections given (=NTEMPT)

INT(8) Indicator for the selection of weighting flux type

(TEMP(i),i=1,12)

Temperature in Kelvin. Zero value is filled for TEMP(i>NTEMPT).

(SIG0(j),j=1,8) Admixture cross-sections for the self-shielding factor tabulation. Zero value is filled for SIG0 (j>NSIGT).

XNU Constant ν-value in thermal range (not used now)

LENGTH Length of data per one-temperature

Member **Kzzmc000** /NGT*(NGT+4)*NTEMPT/ or /4*NGT*NTEMPT/

The following data are repeated for t=1,NTEMPT (See above)

((σ_s(g', g, t), g'=1,NGT), g=1,NGT)

Scattering cross-sections from group g to g'

Note: Some nuclides may not have thermal scattering data. This can be judged by INT(2) above or data length.

(σ_{up}(g, t),g=1,NGT) Up-scattering cross-sections

(σ_c(g, t),g=1,NGT) Capture cross-sections

(σ_t(g, t),g=1,NGT) Total cross-sections

(σ_f(g, t), g=1,NGT) Fission cross-sections

Members **Pzzmc000**, **Qzzmc000**, **Szzmc000**, **Tzzmc000**, and **Uzzmc000**

These members have the same structure as the member Kzzmc000, except that they keep zero values of capture and fission cross-sections.

Member **Fzzmc00r** /NSIGT*NTEMPT*(NGMAXT-NGMINT+1)/
((FTABT(*i*,*t*,*g*),*i*=1,NSIGT),*t*=1,NTEMPT),*g*=NGMINT,NGMAXT)

Self-shielding factors for capture(*r*=C) or fission(*r*=F) cross-sections

Member **Zzzmc000** /NGT*NTEMPT/
((XNU(*g*,*t*),*g*=1,NGT),*t*=1,NTEMPT)

ν-value

3.1.3 Public MCROSS Library [PMCROSS]/ User MCROSS Library [UMCROSS]

Public MCROSS file [PMCROSS] stores point-wise cross-sections data for dominant resonant nuclides at room temperature (~293K), while UMCROSS stores Doppler broadened microscopic hyperfine group cross-sections, which is made by the PEACO routine from the PMCROSS file.

Member name in PMCROSS	Contents
CONT0000	Control information of the library
C*zzm*0000	Control information for the nuclide *zzm* of temperature tagged *t*
F*zzmr*000	Point-wise cross-sections for the nuclide *zzm* of reaction *r* (*r*=F for fission, *r*=C for capture, and *r*=E for elastic)

zz	denotes element chemical symbol as described in Sect.8.1,
m	the last digit of mass number to discriminate isotopes (Sect.8.1),
r	one character to indicate reaction type

3.1.4 Effective Microscopic Cross-Section File [MICREF]

The effective microscopic group cross-sections in fast and thermal energy range are stored in MICREF file. The contents are self-shielded group cross-sections as a result of the table-look-up, the IRA or the PEACO calculation.

Member name	Contents
CONT*e*000	Information of energy group structure in the energy range specified by '*e*': *e*=F for fast energy range and =T for thermal energy range
C*zzm*F*bft*	Control information for the nuclide *zzm* for fast energy range
M*zzm*F*bft*	Effective microscopic cross-sections of the nuclide *zzm* for fast energy range
C*zzm*T*bft*	Control member for the nuclide *zzm* for thermal energy range
K*zzm*T*bft*	Effective microscopic cross-sections of the nuclide *zzm* for thermal energy range
C*zzm*F000	Control information for the nuclide *zzm* for fast energy range: applied to non-resonant nuclide
M*zzm*F00*t*	Infinitely diluted microscopic cross-sections of the nuclide *zzm* for fast energy range: applied to non-resonant nuclide
C*zzm*T00*t*	Control member for the nuclide *zzm* for thermal energy range: applied to non-resonant nuclide
K*zzm*T00*t*	Infinitely diluted microscopic cross-sections of the nuclide *zzm* for thermal energy range: applied to non-resonant nuclide
*mmmm*BMIC	Effective microscopic cross-sections at current burn-up step of whole nuclide contained in the material *mmmm*

zz	the element chemical symbol as described in Sect.8.1,
m	the last digit of mass number to discriminate isotopes (Sect.8.1),
c	one alphameric character for the chemical compound state shown in Sect.8.1,
b	one alphameric character for burn-up step indicator as 0,1,2,……,9,A,B,….Z, a,b,…..,z.
f	one alphameric character for the seventh character of material name,
t	the temperature index as shown in Sect.8.1,
mmmm	the first four character of material name.

Member **CONT*e*002** /2*(ng+1)/

ng	ng=NGF for fast, or ng=NGT for thermal groups
(W(*g*),*g*=1,ng)	Weighted lethargy width (asymptotic spectrum for collapsing)
(E(*g*),*g*=1,ng+1)	Energy boundaries (eV)

Member **C*zzm*F*bft*** or **C*zzm*F000** /42/

ICAP	= 0	No capture
	= 1	Capture cross-sections stored
IFISS	= 0	No fission
	= 1	Fission cross-sections stored
IRES	= 0	No resonance parameter (fixed on MICREF)

LTOT Vector length (word unit) of the member `MzzmFbft` or `MzzmF000`

(LTH(*i*),*i*=1,4) Partial vector length which contains the *i*-th scattering matrix.

(LA(*i*),*i*=1,4) The lowest group number of the energy range where the *i*-th scattering occurs.

(LD(*i*),*i*=1,4) Number of energy groups to which the slowing-down occurs in the *i*-th scattering.

IFS Index for self-shielding factor tables

= 0 No shielding factor (fixed on MICREF)

IFTR, IFC, IFF, IFE, and IFER

Index for self-shielding factor for partial reactions: transport, capture, fission, elastic and elastic removal. Every item for self-shielding factor is set to zero as ineffective on MICREF file.

NGMIN and NGMAX

The highest and lowest energy group for self-shielding factor tabulation. These items are ineffective on MICREF file.

NSIG Number of background cross-sections for tabulation. Ineffective on MICREF

NTEMP Number of temperatures for tabulation. Ineffective on MICREF

AMASS, SIGP, and SIGC0

Properties of the nuclide: not used on MICREF.

(TEMP(*i*),*i*=1,4)

Temperatures for tabulation, not used on MICREF

(SIG0(*i*),*i*=1,8) Background cross-sections, not used on MICREF

IPL Order of elastic scattering.

Member **`MzzmFbft`** or **`MzzmF000`** Fast neutron scattering matrices /LTOT/

(CAPT(*g*),*g*=1,NGF)

Capture cross sections if ICAP=1.

(FISS(*g*),*g*=1,NGF)

Fission cross-sections if IFISS=1.

(FNU(*g*),*g*=1,NGF)

Fission neutron yield per fission (ν) if IFISS=1.

(FSPC(*g*),*g*=1,NGF)

Fission neutron spectrum (χ) if IFISS=1.

(TR(*g*),*g*=1,NGF)

Transport cross-sections

(WEIGHT(g),g=1,NGF)

Lethargy widths weighted by the asymptotic neutron spectrum

(ELAS(g),g=1,NGF)

Total elastic cross-sections

(N-N(g),g=1,LTH(1))

Inelastic scattering matrix of the length LTH(1) = (LD(1)+1)*LA(1)

(N2N(g),g=1,LTH(2))

N2N scattering matrix of the length LTH(2) = (LD(2)+1)*LA(2)

(ELP0(g),g=1,LTH(3))

Elastic P_0 scattering matrix of the length LTH(3) = (LD(3)+1)*LA(3)

(ELP1(g),g=1,LTH(4))

Elastic scattering P_1 matrix of the length LTH(4) = (LD(4)+1)*LA(4)

Member **`CzzmTbft`** or **`Czzmc00t`** Control for thermal data /30/

INT(1) = 0 non fissile

= 1 fissile

INT(2) $= \sum_{1}^{7} \mathrm{IM}(i)$

IM(1) =0 Member `KzzmTbft` (or `Kzzmc00t`) does not include P_0 scattering matrix (but only five vectors of up-scattering capture, total, fission and ν)

IM(2)=2 Member `KzzmTbft` (or `Kzzmc00t`) includes P_0 scattering matrix

IM(3)=4 Member `KzzmTbft` (or `Kzzmc00t`) includes P_1 scattering matrix

IM(4)=8 Member `KzzmTbft` (or `Kzzmc00t`) includes P_2 scattering matrix

IM(5)=16 Member `KzzmTbft` (or `Kzzmc00t`) includes P_3 scattering matrix

IM(6)=32 Member `KzzmTbft` (or `Kzzmc00t`) includes P_4 scattering matrix

IM(7)=64 Member `KzzmTbft` (or `Kzzmc00t`) includes P_5 scattering matrix

INT(3) through INT(6) Not used

INT(7) Number of temperatures for which cross-section is given. (=1 fixed on MICREF)

INT(8) Not used

INT(9) Temperature (K)

INT(10) through INT(30) Not used

Member **KzzmTbft** or **Kzzmc00t** /NGT*(NGT+5) or /5*NGT/

((σ_s (g,g'),g'=1,NGT),g=1,NGT)

P_0 scattering matrix $\sigma_{s,g\to g'}$ if INT(2)>0

Note: Some nuclides may not have thermal scattering data.

(σ_{up} (g),g=1,NGT)

Up-scattering cross-sections

(σ_c (g),g=1,NGT)

Capture cross-sections

(σ_t (g),g=1,NGT)

Total cross-sections

(σ_f (g),g=1,NGT)

Fission cross-sections

(ν (g),g=1,NGT)

Neutron yields per fission in thermal range

Member ***mmmm*BMIC** /MAXNG*6*MMK/

(((σ_{eff} (g,x,i),g=1,MAXNG),x=1,6),i=1,MMK)

where σ_{eff} (g,x,i) is the effective microscopic cross-sections of energy group g, reaction x, nuclide i.

MAXNG is the maximum number of groups (=107) fixed by the parameter in a include file of the SRAC sources. If g-value exceeds the number of fine groups, null values are filled.

The reaction types are σ_c by x=1, σ_f by x=2, σ_e (elastic) by x=3, σ_{er} (elastic removal) by x=4, $\sigma_{n,2n}$ by x=5 and $\nu\sigma_f$ by x=6.

MMK is the number of the whole nuclides contained in the material if IC20=0 (cf. Sect.2.2) is specified. Otherwise (burn-up calculation), MMK is the number of whole depleting nuclides implicitly determined by the burn-up chain model even at the zero burn-up step. As this member has no burn-up tag, the cross-section values are updated by those at the current burn-up step.

3.1.5 Fine Group Macroscopic Cross-Section File [MACROWRK]

The macroscopic cross-sections by material and those by X-Region obtained by homogenization are stored in the fine group macroscopic cross-sections file (MACROWRK) with the fine group structure.

Member name	Contents
CONT*e*002	Energy group structure for the energy range specified by *e-tag*
mmmmebfp	Cross-sections of material *mmmm*
*mmmmebf*M	(n,2n) cross-sections of material *mmmm*
*mmmmebf*Y	Delayed neutron data of material *mmmm*
caseebxp	Cross-sections of X-Region *x*
*caseebx*M	(n,2n) cross-sections of X-Region *x*
*caseebx*Y	Delayed neutron data of X-Region *x*

mmmm	First four characters of material name (MTNAME in Sect.2.9),
case	Case name (See Sect.2.9),
e	Energy range indicator: *e*=F for fast, *e* =T for thermal, *e* =A for whole energy range,
b	one alphanumeric character for burn-up step indicator as 0,1,2,……,9,A,B,….Z,a,b,….,z. For non-depleting material in burn-up problem or the material with composition in non-burn-up problem, the sixth character of material name is given.
f	one alphanumeric character for the seventh character of material name.
x	one alphanumeric character for X-Region number (1,2,……..,9,A,B,….Z) is given.
p	Legendre component indicator.
	p=2: P_0 component with transport correction,
	p=3: P_1 component,
	p=4: P_0 component without transport correction.
	p=5: P_2 component (for the material including nuclides with higher order P_L data)
	p=6: P_3 component (for the material including nuclides with higher order P_L data)
	p=7: P_4 component (for the material including nuclides with higher order P_L data)
	p=8: P_5 component (for the material including nuclides with higher order P_L data)

Member **CONT*e*002** /2*(Number of groups+1)/

ng Number of energy groups (depends on *e*-tag)

(W(*g*),*g*=1,ng)

Weighted lethargy widths that may be utilized in collapsing the group structure.

(E(*g*),*g*=1,ng+1)

Energy boundaries (eV) starting at the highest energy

Member **mmmmebfp** or **caseebxp** /10*ng+$\sum_{g=1}^{ng}$LGV(g)/

The member keeps a complete set of group cross-sections in a one-dimensional array. We shall show below a partial vector corresponding to a energy group g.

DO g=1,ng (ng: in `CONTe000`)

1 LSS(g) Position of the self-scatter on the scattering vector

2 LGV(g) Length of the scattering vector

3 $\Sigma_{\upsilon}(g)$ Constant related to neutron velocity (υ_g) for the calculation of point kinetics parameters

$$\Sigma_{\upsilon,g} \equiv \sqrt{\frac{1}{\overline{E}_g}} = \sqrt{\frac{1}{\left(E_g(eV) + E_{g+1}(eV)\right)/2}},$$

$$\upsilon_g(m/\sec) = \sqrt{\frac{2\times 1.60219E-19}{m_n(kg)}}\frac{1}{\Sigma_{\upsilon}} = 13831.68\times\frac{1}{\Sigma_{\upsilon}}$$

4 $\Sigma_f(g)$ Fission cross-section

5 $\nu\Sigma_f(g)$ Production cross-section

6 $\Sigma_t(g)$ Total (p=2) or transport (p=4) cross-section

7 $\chi(g)$ Fission neutron yield

8 D1(g) Diffusion coefficient 1

9 D2(g) Diffusion coefficient 2

10 $\Sigma_a(g)$ Absorption cross-section followed by the scattering vector

1	$\Sigma_{g\to g1}$	where $g1$=g-LSS(g)+1
2	$\Sigma_{g\to g1+1}$	
3	$\Sigma_{g\to g1+2}$	
	-	
	-	
LSS(g)	$\Sigma_{g\to g}$	
	-	
	-	
LGV(g)	$\Sigma_{g\to g2}$	where $g2$=g+LGV(g)-LSS(g)

END DO (The above organization is repeated ‘ng’ times in the whole vector.)

Member **mmmmebfM** or **caseebxM** /10*ng+$\sum_{g=1}^{ng}$LGV(g)/

The (n,2n) matrix data for the mixture or the homogenized cell. The data organization is the same as for the standard member *mmmmebfp* or *caseebxp* while null values are filled in the position of Σ_{υ} through Σ_{a}.

Member **mmmmebfY** or **caseebxY** /3*ng*IFM/

The delayed neutron data for the mixture or the homogenized cell used for the one point kinetics parameter calculation in CITATION (cf. Sect.2.8). IFM is number of delayed neutron families: usually IFM=6, and IFM=15 if D_2O is concerned.

(BVFSIG(j,g),j=1,IFM),g=1,ng)

The parameter for delayed neutron fraction by family j

$$\mathrm{BVFSIG}(j,g)=\sum_{n}\beta_n^j \nu\sigma_{f,g}^n N^n \quad (n\text{: nuclide})$$

(χ_d(j,g),j=1,IFM),g=1,ng)

Delayed neutron spectrum by family j

(BVLSIG(j,g),j=1,IFM),g=1,ng)

The parameter for decay constant by family j

$$\mathrm{BVLSIG}(j,g)=\sum_{n}\frac{\beta_n^j \nu\sigma_{f,g}^n N^n}{\lambda_j^n} \quad (n\text{: nuclide})$$

3.1.6 Coarse Group Macroscopic Cross-section File [MACRO]

The macroscopic cross-sections by material and by X-Region collapsed by calculated or asymptotic spectrum are stored in the coarse group macroscopic cross-sections file (MACRO) in the coarse (few) group structure.

Member name	Contents
CONTe000	Energy group structure for the energy range specified by *e-tag*
mmmmebfp	Cross-sections of material *mmmm*
*mmmmebf*N	(n,2n) cross-sections of material *mmmm*
*mmmmebf*Z	Delayed neutron data of material *mmmm*
caseebxp	Cross-sections of X-Region *x*
*caseebx*N	(n,2n) cross-sections of X-Region *x*

*caseebx*Z Delayed neutron data of X-Region *x*
*case*BNUP Result of burn-up calculation for depleting materials
*case*DN*x*T Result of burn-up calculation for by X-Region *x*
*case*HT*jj* Intermediate step information to restart burn-up calculation

****

mmmm First four characters of material name (MTNAME in Sect.2.9).
case Case name (in Sect.2.9).
e Energy range indicator: *e*=F for fast, *e*=A for whole energy range.
b Burn-up step indicator (0, 1, 2,…….., 9,A,B,…..,Z,a,b,……,z).
For non-depleting material in burn-up problem or the material with composition in non-burn-up problem, the sixth character of material name is given.
f The seventh character of material name is given.
x X-Region number (1,2,……..,9,A,B,….Z) is given.
p Legendre component indicator
p=0: P_0 component with transport correction for the members processed after isotropic calculations by PIJ, TUD or CITATION,
P_0 component without transport correction for the members processed after anisotropic calculations by ANISN or TWOTRAN,
p=1: P_1 component for the members processed after anisotropic calculations by ANISN or TWOTRAN.
jj Two digit number corresponding to burn-up steps (*jj*=00,01,02,03….)

****

The contents and structures of the members on MACRO file are consistent with those on MACROWRK file except for the difference of energy group structure.

MACRO		MACROWRK	
CONT*e*000		CONT*e*002	
mmmmebfp	(*p*=0,1)	*mmmmebfp*	(*p*=2,3,4,5,6,7,8)
*mmmmebf*N		*mmmmebf*M	
*mmmmebf*Z		*mmmmebf*Y	
caseebxp	(*p*=0,1)	*caseebxp*	(*p*=2,3,4)
*caseebx*N		*caseebx*M	
*caseebx*Z		*caseebx*Y	

****

The members related to burn-up calculation are usually written on MACRO file. In the case without group collapsing, they are stored on MACROWRK file. Principal results of burn-up calculation are kept in the members *case*BNUP and *case*DN*x*T. Especially, the member *case*DN*x*T keeps the homogenized composition of depleting isotopes at every burn-up step when the cross-sections are calculated. This tabulation will be utilized in the auxiliary code COREBN.

Member ***caseBNUP*** Material-wise burn-up information

1 NOWSTP Number of burn-up steps including the initial step.
If the burn-up calculation is completed, NOWSTP=1+IBC1 (Sect.2.11).

2 NTNUC Total number of depleting nuclides

3 NZON Number of depleting materials in a cell

4 IDUM4 = 0 not used

5 IDUM5 = 0 not used

6 IDUM6 = 0 not used

7 IDUM7 = 0 not used

8 IDUM8 = 0 not used

9 IDUM9 = 0 not used

10 IDUM10 = 0 not used

11 CASE Case name (A4)

12 STDNUC Nuclide ID (A4) used for the measure of depletion fraction (cf. Block-4 of Sect.2.11, 'XU05' is defaulted when IBC2>0 (cf. Block-1 of Sect.2.11)

(TITLE(*i*),*i*=1,18)
Comment of 72 characters (18A4)

(MTNM(*m*),*m*=1,NZON)
Former half of depleting material names specified in Sect.2.9. NZON is number of depleting materials (by M-Region)

(MTYP(*m*),*m*=1,NZON)
Type of depleting materials
= 1 Fissionable material (e.g. UO_2)
= 2 Non-fissionable material (e.g. Gd_2O_3)

(VOLDPZ(*m*),*m*=1,NZON)
Volumes of depleting materials (cm^3)

(NUCLID(*i*),*i*=1,NTNUC)
Index of nuclide name by four characters. The first character is set to 'X', the succeeding three characters denote *zzm* (e.g. XU05, XPU9).

(DAYS(*j*),*j*=1,NOWSTP)
Accumulated burn-up days (unit day) by step *j*

The step number j=1,2,3,4,…,10,11,12,… corresponds to the burn-up tag of the member in PDS b= 0,1,2,3,…,9,A,B…. , respectively.

(EXPST(j),j=1,NOWSTP)

Accumulated burn-up (MWd/t) of whole cell

(U235F(j),j=1,NOWSTP)

Depletion fraction (%) of nuclide STDNUC (cf. Block-4 of Sect.2.11)

U-235 is defaulted when IBC2>0 (cf. Block-1 of Sect.2.11)

U235F(j) $\leq$ 100 (negative value may be appeared for the nuclide increasing with burn-up, e.g. blanket fuel)

(AKEFF(j),j=1,NOWSTP)

Effective multiplication factor by step. AKEFF(NOWSTP)=0.0, because flux (eigenvalue) calculation is not done at the last step.

(AKINF(j),j=1,NOWSTP)

Infinite multiplication factor by step. AKINF(NOWSTP)=0.0

(INSCR(j),j=1,NOWSTP)

Instantaneous conversion ratio by step. INSCR(NOWSTP)=0.0

(INTCR(j),j=1,NOWSTP)

Integrated conversion ratio by step. INTCR(NOWSTP)=0.0

(POWERL(j),j=1,NOWSTP)

Thermal power per unit length of cell (MWt/cm) by step.

POWERL (NOWSTP)=0.0

In the constant flux calculation, POWER($j \leq 1$) are calculated by code.

(FLXNRM(j),j=1,NOWSTP)

Normalizing factor of neutron flux by step. FLXNRM(NOWSTP)=0.0.

Even in the restart calculation under constant flux level, the flux level is set to FLXNRM(1) throughout the exposure.

((POWRZN(j,m),j=1,NOWSTP),m=1,NZON)

Power density (MW/cm^3) by step j by depleting material m

((EXPSZN(j,m),j=1,NPWSTP),m=1,NZON)

Burn-up (MWd/t) by step by depleting material

In the case of MTYPX(m)=2, time integrated absorption rate (n/cm^3) is given.

((HMINV(j,m),j=1,NOWSTP),m=1,NZON)

Heavy metal inventory (ton/cm^3) by step by depleting material

Initial inventory in the restart calculation is given by

$$\sum_{m} \{\text{HMINV}(1,m)*\text{VOLDPZ}(m)\}$$

((RLHT(*j*,*m*),*j*=1,NOWSTP), *m*=1,NZON)

Heat generation (Joule/fission) by step by depleting material

((YDXE(*j*,*m*),*j*=1,NOWSTP),*m*=1,NZON)

Fission yield of Xe-135 by step by depleting material

((YDIO(*j*,*m*),*j*=1,NOWSTP), *m*=1,NZON)

Fission yield of I-135 by step by depleting material

((YDSM(*j*,*m*),*j*=1,NOWSTP),*m*=1,NZON)

Fission yield of Sm-149 by step by depleting material

((YDPM(*j*,*m*),*j*=1,NOWSTP),*m*=1,NZON)

Fission yield of Pm-149 by step by depleting material

((DENSTY(*j*,*i*,*m*),*j*=1,NOWSTP),*i*=1,NTNUC),*m*=1,NZON

Atomic number density (10^{24} n/cm^3) by step by nuclide by depleting material

(((SIGXE(*g*,*j*,*m*),*g*=1,ng),*j*=1,NOWSTP),*m*=1,NZON)

Few group microscopic capture cross-sections of Xe-135 by group *g* by step *j* by depleting material *m*. If no collapsing is done, fine group cross-sections are given.

(((SIGIO(*g*,*j*,*m*),*g*=1,ng),*j*=1,NOWSTP),*m*=1,NZON)

Few group microscopic capture cross-sections of I-135 by group by step by depleting material.

(((SIGSM(*g*,*j*,*m*),*g*=1,ng),*j*=1,NOWSTP),*m*=1,NZON)

Few group microscopic capture cross-sections of Sm-149 by group by step by depleting material. If no collapsing is done, fine group cross-sections are given.

(((SIGPM(*g*,*j*,*m*),*g*=1,ng),*j*=1,NOWSTP),*m*=1,NZON)

Few group microscopic capture cross-sections of Pm-149 by group by step by depleting material. If no collapsing is done, fine group cross-sections are given.

Member **_caseDNxT_** Homogenized burn-up information

Contents of the member are same as those of the member *case*BNUP, however, all data in this member is homogenized in the *x*-th X-Region.

1 NOWSTP Number of burn-up steps including the initial step.

If the burn-up calculation is completed, NOWSTP=1+IBC1 (Sect.2.11).

2 NTNUC Total number of depleting nuclides

3 ng Number of few groups, If no collapsing is done, number of fine groups is given

4 NGT Number of few thermal groups. If no collapsing is done, number of fine thermal groups is given.

5 IDUM5 = 0 Not used

6 IDUM6 = 0 Not used

7 IDUM7 = 0 Not used

8 IDUM8 = 0 Not used

9 IDUM9 = 0 Not used

10 IDUM10 = 0 Not used

11 CASE Case name (A4)

12 STDNUC Nuclide ID (A4) used for the measure of depletion fraction

XU05 is defaulted

13 MTYPX Type of depleting materials

= 1 Fissionable material (usual fuel)

= 2 Non-fissionable depleting material (e.g. Gd_2O_3)

14 VOLX Volume of this X-Region (cm^3)

(NUCLID(i),i=1,NTNUC)

Nuclide ID by A4. The first character is set to 'X', the succeeding three characters denote zzm (e.g. XU05, XPU9)

(POWERX(j),j=1,NOWSTP)

Average power density (MW/cm^3) of this X-Region by step

(EXPSX(j),j=1,NPWSTP)

Average accumulated burn-up (MWd/t) by step

In the case of MTYPX=2, time integrated absorption rate (n/cm^3) is given.

(U235FX(j),j=1,NOWSTP)

Depletion fraction (%) of nuclide STDNUC (U-235 is defaulted)

U235FX(j) $\leq$ 100.0

(HMINVX(j),j=1,NOWSTP)

Heavy metal inventory (ton/cm^3) of this X-Region by step

(RLHTX(j),j=1,NOWSTP)

Heat generation (Joule/fission) of this X-Region by step

(YDXEX(j),j=1,NOWSTP)

Fission yield of Xe-135 by step

(YDIOX(*j*),*j*=1,NOWSTP)

Fission yield of I-135 by step

(YDSMX(*j*),*j*=1,NOWSTP)

Fission yield of Sm-149 by step

(YDPM(*j*),*j=1*,NOWSTP)

Fission yield of Pm-149 by step

((DENSTY(*j*,*i*),*j*=1,NOWSTP),*i*=1,NTNUC)

Atomic number density (10^{24} n/cm^3) by step by nuclide

((AFISS(*g*,*j*),*g*=1,ng),*j*=1,NOWSTP)

Few group macroscopic absorption cross-sections of fissile nuclides by group by step.

((CFERT(*g*,*j*),*g*=1,ng),*j*=1,NOWSTP)

Few group macroscopic capture cross-sections of fertile nuclides by group by step.

((SIGXEX(*g*,*j*),*g*=1,ng),*j*=1,NOWSTP)

Few group microscopic capture cross-sections of Xe-135 by group by step

((SIGIOX(*g*,*j*),*g*=1,ng),*j*=1,NOWSTP)

Few group microscopic capture cross-sections of I-135 by group by step

((SIGSMX(*g*,*j*),*g*=1,ng),*j*=1,NOWSTP)

Few group microscopic capture cross-sections of Sm-149 by group by step

((SIGPMX(*g*,*j*),*g*=1,ng),*j*=1,NOWSTP)

Few group microscopic capture cross-sections of Pm-149 by group by step

Member ***case*HT*jj*** member for restart burn-up calcuation

This member is written at the end of every burn-up step (*jj*=00, 01, 02, ….). This keeps the burn-up information of the step to make the members *case*BNUP and *case*DT*x*T. At the end of whole steps, the code edits these restart members and creates the members *case*BNUP and *case*DTxT. Therefore, even if an abnormal termination occurs, the restart is available by using the members *case*HT*jj*. As the contents of this member are included in the members *case*BNUP and *case*DN*x*T, description is skipped.

3.1.7 Flux File [FLUX]

The neutron fluxes integrated spatially in 'R-Region' (PIJ), in 'zone' (ANISN), in 'coarse mesh zone' (TWOTRAN), in 'region' (TUD) or in 'zone' (CITATION) and those integrated in X-Region are stored in FLUX file. For plotting and homogenization purpose, the volumes of each spatial region are also written. The following six kinds of members are treated in this file.

Member name	Contents
CONT*e*00*p*	Energy group structure for the energy range specified by *e-tag*
*case*eeb0*p*	Neutron fluxes by R-Region by group
*case*eb*x*p	Neutron fluxes of X-Region *x* by group
*case*eeVOL	Volumes of R-Regions: *e*=F or T in the fixed source mode, *e*=A in the eigenvalue mode
*case*SVOL	Volumes of T-Regions in PIJ fixed source problem mode
*case*AbS2	Fixed boundary source (fed by user)
mmmmAbS2	Neutron spectrum for collapsing cross-sections of isolated materials (fed by user)

case	Case name (in Sect.2.9).
e	Energy range indicator: *e*=F for fast, *e*=T for thermal, *e*=A for whole energy range.
b	Burn-up step indicator (0, 1, 2,…….., 9,A,B,…..,Z,a,b,…..,z). For non-depleting problem, '0' is given.
x	X-Region number (1,2,……..,9,A,B,….,Z) is given.
p	Indicator for energy group structure; *p*=0 for coarse (few) group, *p*=2 for fine group

Member **CONT*e*00*p*** /2*(ng + 1)/

ng number of energy group (depending on *e*-tag)

ng=NEF (or NERF) for fast, ng=NET (or NERT) for thermal or ng=NEF+NET (or NERF+NERT) for whole energy range

See Block-6 of Sect.2.2 for NEF, NET, NERF, NERT.

(W(*g*),*g*=1,ng)

Weighted lethargy width (asymptotic spectrum for collapsing)

(E(*g*),*g*=1,ng+1)

Energy boundaries (eV) starting at the highest energy

Member ***case*eeb0*p*** /NRR*ng/

(PHI(*i*,*g*),*i*=1,NRR),*g*=1,ng)

Neutron flux multiplied by volume of region *i* and lethargy width of group *g*

(n/cm^2/sec*cm^3), NRR is number of R-Regions.

Member ***caseebxp*** /ng/
(PHIX(*g*),*g*=1,ng)

Neutron flux multiplied by volume of X-Region *x* (n/cm^2/sec*cm^3)

Member ***case*eVOL** (*e*='F' or 'T' if fixed source mode, otherwise ='A') /NRR/
(VOLR(*i*), *i*=1,NRR)

Volume of R-Region *i* (cm^3)

Member ***case*SVOL** /NR/
(VOLT(*i*), *i*=1,NR)

Volume of T-Region *i* (cm^3)

Member ***case*AbS2** /ng (fine-group)/

The spectrum stored in this member will be used as the in-current flux at the outer boundary of the cell. It is used in the fixed source problem specified by IC12=-2 in Sect.2.2. The member has to be prepared before the execution. Data structure is identical with that of the member *caseebxp*.

Member ***mmmm*Abx2** /ng (fine-group)/

The spectrum stored in this member will be used as the weight to collapse the fine-group cross-sections into few-group constants of isolated mixture like reflector material identified by *mmmm*-tag, *b*-tag and *x*-tag. The member has to be prepared before the execution. In usual case, i.e. when this member is not given, the asymptotic spectrum stored in the Public library is used as the weighting spectrum. The user can replace the spectrum by this member.

3.2 I/O Files in Sequential Organization

Here we shall describe the usage of sequential files. Some of them are used in the special routine and some are commonly used. It is organized that even if the logical number of file is identical between in a routine and in common use, any conflict use will not occur.

The following table shows the assignment of logical number to the variable name defined by FORTRAN statements used by routine. Name enclosed by [ ] is the subroutine name to use the unit. Their physical contents are explained by routine.

Table 3.2-1 Logical device number and file format in SRAC

No.	MAIN	PIJ	ANISN	TWOTRAN	TUD	CITATION	RECFM*
01			NT1	NEDIT		IO1	binary
02			NT2	IXMESH		IO2	binary
03	[MACROF]		NT3			IO3	binary
04	NFTOT	[SIGRD]	NT4	NEXTRA			binary
05	[DTLIST]		NIN	NINP			text(80)
06	NOUT1		NOUT1	NOUT			text(137)
08			NT8	NAFLUX			binary
09				LAFLUX		IOFLX	binary
10			NT6,NT7	ISOTXS		IX(77)	binary
11				ISNCON		IX(78)	binary
12				NDUMP1			binary
13				NDUMP2		IX(80)	binary
14				IVMESH		IX(81)	binary
15						IX(82)	binary
16						IX(83)	binary
17						IX(84)	binary
18		[ITER]				IX(85)	binary
19						IX(86)	binary
21		[ITER,FORM, INP3F]					binary
22		[FORM,TEDIT]					binary
26						IX(93)	binary
28						IX(95)	binary
31	[CVMACT]					IX(137)	text(80)
32	NSOUC	[INP3F]	NSOUC	IFIXSR	ISOURC	IX(138)	binary
33	NFIN	[TEDT]	[FINPR]	ITFLUX	IFOUT		binary
49	IOPDS						binary
50	[BURNIN]						text(80)
52	[MICREF, BURNCT]						text(80) binary
81		[OPNBUF]					binary
82		[OPNBUF]					binary
83		[OPNBUF]					binary
84		[OPNBUF]					binary
85		[PIJIN]					binary
89	[PIFLIB]	[PIFLIB]					text(137)
91						IOIN	text(80)
92						[CIT1,2]	binary
93	[BURNUP]						text(80)
95	[DTLIST]						text(80)
96	[PEACO]						binary
97	[BURNRW]						binary
98	[BURNUP]						text(137)
99	NOUT2						text(137)

*Record format (text length)

3.2.1 Common PS Files

The following PS files are commonly used in SRAC

Logical unit		Contents
03		Scratch unit for macroscopic cross-section formation
05	NIN	Standard input unit
06	NOUT1	Standard output unit for calculation logs, error or warning messages.
31		Scratch file to convert cross-sections of PDS into CITATION format
32		Scratch file to feed the fixed source distribution : formed in FSOURC or TSOURC routine to any of transport routine
33		Scratch file used to transfer the neutron fluxes solved by any of the transport routine to MIXX routine
49		Unit to open/close PDS member
50		Input file to keep the chain scheme for burn-up calculation
		Scratch file to transfer the information from the preparation step of burn-up calculation to the execution step
52		Scratch file to transfer the effective microscopic cross-sections from MICREF step to BURNUP step and to the reaction rate calculation.
89		Postscript file for plotting (in PEACO or PIJ)
93		Scratch unit used in the cell burn-up calculation
95		Scratch unit used for echo of input data
96		Scratch unit used in the PEACO calculation
97		Scratch unit used in the cell burn-up calculation
98		Print unit of summary table in the cell burn-up calculation
99	NOUT2	Print unit for calculated results

3.2.2 PS files for PIJ

The PS files used for PIJ (other than common PS files) are as follows.

Logical unit	Contents
04	Scratch unit for total cross-section
21	Collision probabilities storage
22	Directional collision probabilities storage (required if IC17=2)
32	Interface file for fixed source
33	Interface file for fluxes
81	Scratch unit for path table
82	Scratch unit for path table
83	Scratch unit for path table
84	Scratch unit for path table

85	Tabulated Bickley function

****

3.2.3 PS files for ANISN

The PS files used for ANISN (other than common PS files) are as follows.

Logical unit		Contents
01	NT1	Flux and current storage unit (not used)
02	NT2	Flux and current storage unit in the previous iteration (not used)
03	NT3	Scratch unit for cross-section and fixed source storage (not used if IDAT1 is set to zero)
04	NT4	Scratch unit for normalization of source
10	NT6	Interface file for macroscopic cross-sections
08	NT8	Weighted cross-section unit
32	NSOUC	Interface file for fixed source
33	NFLUX	Flux and current each in one record

****

3.2.4 PS files for TWOTRAN

The PS files used for TWOTRAN (other than common PS files) are as follows.

Logical unit		Contents
01	NEDIT	Edit input storage
02	IXMESH	X-Region output storage to SRAC
04	NEXTRA	Scratch unit
08	NAFLUX	Angular flux by group
09	LAFLUX	Output form of angular flux
10	ISOTXS	Input for cross-sections fed by SRAC main
11	ISNCON	Output for SN constants
12	NDUMP1	First restart dump unit
13	NDUMP2	Second restart dump unit
14	IVMESH	Zone output storage to SRAC main
32	IFIXSR	Input of inhomogeneous source fed by SRAC main
33	ITFLUX	Output form of total flux

****

3.2.5 PS files for TUD

The PS files used for TUD (other than common PS files) are as follows.

Logical unit		Contents
32	ISOURC	Input of inhomogeneous source fed by SRAC main
33	IFOUT	Output unit of flux distribution

3.2.6 PS files for CITATION

The PS files used for CITATION (other than common PS files) are as follows.

Logical unit		Contents
01	I01	Scratch unit, always required.
02	I02	Scratch unit, always required.
03	I03	Scratch unit, always required.
09	IOFLX	Used to store forward neutron flux map by option. See NGC6 in section 001. Also used to store forward and adjoint fluxes for use in perturbation calculation. Required if NGC6>0, or if the adjoint problem is specified.
10	IX(77)	Scratch unit, always required.
11	IX(78)	Scratch unit, always required.
13	IX(80)	Output unit for restart, required if NGC2 and/or NGC3 >0.
14	IX(81)	Scratch unit to store macroscopic cross-sections, always required.
15	IX(82)	Scratch unit to store equation constants if I/O during the iterative calculation is necessary. This is the unit to which the high speed I/O is effective.
16	IX(83)	Scratch unit, always required.
17	IX(84)	Scratch unit to store space-energy fixed source, and used to save point neutron source.
18	IX(85)	Scratch unit used in perturbation calculation
19	IX(86)	Scratch unit, always required.
26	IX(93)	Scratch unit used in perturbation calculation
28	IX(95)	Scratch unit used in perturbation calculation
31	IX(137)	Interface file to receive macroscopic cross-sections
32	IX(138)	Power density and heat to coolant, if required.
91	IOIN	Scratch unit to transfer input data in text data from input process CIT1 step to execution CIT2 step
92		Scratch unit to transfer reaction rate information in text data from CIT1 step to CIT2 step

3.3 Burn-up Chain Library

There are several burn-up chain library files in text format. Each file keeps a burn-up chain scheme (model) where the decay chains and constants are described. The user can choose any of them considering the reactor type and his purpose, or he can edit his own chain scheme if necessary.

Table 3.3-1 Available burn-up chain models[29)]

Type of burn-up chain models (main purpose)	Name of chain model (=file name of burn-up chain data)	
	for thermal reactors	for fast reactors
Standard chain model (nuclear calculations)	u4cm6fp50bp16T th2cm6fp50bp16T	u4cm6fp50bp16F th2cm6fp50bp16F
General-purpose chain model (PIE analyses and so on)	u4cm6fp104bp12T	
Detailed chain model (validation of other chain models)	th2cm6fp193bp6T	th2cm6fp193bp6F

values of fission yield and isomeric ratio are different between models for thermal and fast reactors

file name [SRAC/lib/burnlibT/*]	Contents
u4cm6fp50bp16T/F	The member describes the model which includes 21 heavy nuclides starting from U-234 to Cm-246 (Fig.3.3-1) and 49 explicit FPs and one pseudo FP (Fig.3.3-3). Burnable poisons such as gadolinium and boron can be treated. This is a standard model for nuclear analyses of the core with UO_2 and/or MOX fuel.
th2cm6fp50bp16T/F	This model includes 28 heavy nuclides from Th-232 to Cm-246 (Fig.3.3-2) and the same treatment to FPs and burnable poisons as that of u4cm6fp50bp16T/F. When U-233 and Thorium are involved or accurate evaluation of radio-toxicity by minor actinides is required, this model is suitable.
u4cm6fp104bp12T	This model includes 103 explicit FPs and one pseudo FP (Fig.3.3-4). It is optimized not only from the viewpoint of nuclear analyses but also for analyses of spent fuel composition.
th2cm6fp193bp6T/F	This model includes 193 explicit FPs and no pseudo. It is the most detailed FP chain model for SRAC developers (Fig.3.3-5) to validate other chain models and create pseudo FP cross-sections.

The structure of burn-up chain model is as follows. Any comment line can be inserted with '*'

at the first column.

Block-1-1	Number of nuclides	/5/
1 LNMAX	Number of total nuclides registered. Heavy nuclides, FP nuclides and burnable poison nuclides should be included. Non-depleting nuclides may be included, however, they are ineffective in the burn-up calculation.	
2 NMAX	Number of nuclides related to depletion and/or decay (usually LNMAX=NMAX)	
3 NFIS	Number of fissionable nuclides (heavy nuclides)	
4 NPAR	Maximum number of parent nuclides from which a depleting nuclide is produced (cf. NCH in Block-3-1)	
5 NYLDTY	Number of types of FP yield data (cf. Block-4)	

Block-1-2	General constants	/4/
1 ANMU	Conversion factor to get atomic mass in amu unit for AMASS(*i*) in Block-2 If AMASS(*i*) is given in amu, enter 1.0.	
2 AVOGA	Avogadro number (6.0221358E+23 n/mol)	
3 EVTOJ	Conversion factor to get energy in *Joule* unit for energy in eV unit (1.160219E-19 J/eV)	
4 GASCON	Gas constant (8.3148 J/mol/K)	

DO *i*=1,LMAX	<Repeat Block-2 for *i*=1,LMAX times>	
Block-2	Nuclide list (Free format for the last 7 data in columns 19-80)	/A8,2X,A8,7/
1 IHOL(*i*)	Nuclide ID by 8 characters (e.g. `U-235___`)	
2 SRACID(*i*)	Nuclide ID by 8 characters in SRAC format: X*zzmc*`---` (e.g. `XU050001`) The last 3 characters are ineffective.	
3 NCODE(*i*)	Code number of nuclide (enter after column 19) Number is arbitrary, but not duplicate with that of another nuclide. e.g. the definition ‘atomic number + mass number + (0: ground / 1: exited)’ like 922350 gives reasonable numbering.	
4 AMASS(*i*)	Mass of nuclide Unit is arbitrary (currently neutron mass unit is used). Multiplied by ANMU in Block-1-2, it makes mass in *amu* unit.	
5 IFISS(*i*)	Attribute of nuclide > 1 heavy nuclide (fissionable) related to instantaneous conversion ratio	

= 1 heavy nuclide (fissionable) not related to instantaneous conversion ratio

= 0 FP (burnable poison nuclide is included, if it has fission yield)

= -1 nuclide without cross-section data (decay is considered)

≤ -10 non-FP nuclide used for burnable poison (without fission yield)

Heavy nuclides assigned as IFISS(*i*)>1 by this item are used for the default definition of instantaneous conversion ratio. Unless the user redefines the conversion ratio by the option IBC5=1 in Sect.2.11, the ratio is defined as follows;

The instantaneous conversion ratio

=(production rate of fissile nuclides)/(depletion rate of fissile nuclides)

≈ (capture rate of fertile nuclides)/(absorption rate of fissile nuclides),

where IFISS(*i*)=2 should be given to fertile nuclides for the numerator, and IFISS(*i*)=3 to fissile nuclides for the denominator.

6 IRES(*i*) Indicator of resonant nuclide (cf. Sect.2.9)

= 0 non-resonant nuclide

= 2 resonant nuclide

7 EFISS(*i*) Emission energy per fission (MeV/fission)

8 ECAP(*i*) Emission energy by (n, γ) reaction (MeV/emission)

Give zero value (ineffective) for ECAP, because only EFISS is treated as heat generation in the current SRAC.

9 FACT2N(*i*) For validation purpose, (n,2n) reaction rate is multiplied by FACT2N(*i*). Set 1.0 usually.

END DO <end of repetition for Block-2>

DO *j*=1,NMAX <Repeat Block-3 for *j*=1,NMAX times>

Block-3-1 Decay data /A8,I2,E10.3,A2/

1 NUCL(*j*) Nuclide ID by 8 characters as specified by IHOL in Block-2 of nuclide related to depletion and/or decay

2 NCH(*j*) Number of parent nuclides of NUCL(*j*)

NCH(*j*) should be less or equal to NPAR in Block 1-1.

3 HALFT(*j*) Half-life of NUCL(*j*) in unit specified by the next item)

4 TUNIT(*j*) Unit of HALFT(*j*) by 8 (or less) characters (first character is effective)

= ‘SECONDS’ second

= ‘MINUTES’ minutes

= ‘HOURS’ hours

= ‘DAYS’ days

= ‘YEARS’ years

DO *k*=1,NCH(*j*) <Repeat Block-3-2 for *k*=1,NCH(*j*) times>

Block-3-2 Decay path from parent nuclides /A3,2X,A8,2X,E12.5/

1 NUCLP(*k*) Nuclide ID by 8 characters as specified by IHOL in Block-2 of a parent nuclide of NUCL(*j*)

2 NBIC(*k*) Decay type from NUCLP(*k*) to NUCL(*j*) by 8 (or less) characters.

First five characters are effective.

= ‘BETA-‘ β^- decay

= ‘IT’ isomeric transition

= ‘BETA+’ β^+ decay

= ‘EC’ orbital electron capture

= ‘ALPHA’ α decay

= ‘CAPTURE’ (n,γ) reaction

= ‘2N’ (n,2n) reaction

= ‘DELAYED’ delayed neutron emission

3 PBIC(*k*) Branching ratio from NUCLP(*k*) to NUCL(*j*) of this decay

END DO <end of repetition for Block-3-2>

END DO <end of repetition for Block-3>

DO *m*=1,NYLDTY <Repeat Block-4 for *m*=1,NYLDTY times>

Block-4-1 /A8,2/

1 NAMYLD(*m*) ID name of *m*-th type FP yield data by 8 (or less) characters

(e.g. ‘YU235T’ for U-235 thermal fission)

2 NYNUCL(*m*) Number of heavy nuclides to commonly use *m*-th type FP yield data

3 NFP(*m*) Number of FP nuclides included in *m*-th type FP yield data

Block-4-2 /5(A8,2X)/

(NAMFIS(*i*), *i*=1,NYNUCL(*m*))

Nuclide ID names appearing in IHOL in Block-2 of heavy nuclides (IFISS>0) to commonly use *m*-th type FP yield data in 5*(A8,2X) format

DO *n*=1,NFP(*m*) <Repeat Block-4-3 for *n*=1,NFP(*m*) times>

Block-4-3 /A8,1/

NAMFP(*n*) Nuclide ID names appearing in IHOL in Block-2 of FP (IFISS=0) included in *m*-th

type FP yield data

YLDFP(*n*) Fission yield of the nuclide of ID name NAMFP(*n*)

END DO <end of repetition for Block-4-3>

END DO <end of repetition for Block-4>

The chain model ‘u4cm6fp50bp16T’ is described as follows;

```
*LNMAX NMAX NFIS NPAR NYLDTY  (FREE FORMAT) for Block-1-1
   87   87   21    4    8
*  ANMU      AVOGA         EVTOJ    GASCON (FREE FORMAT) for Block-1-2
1.008665  6.0221358E+23  1.60219E-19  8.3148
*Registration of Nuclide for Block-2, Repeat LNMAX Times
*IHOL     SRACID  NCODE   AMASS    IFISS  IRES   EFIS    ECAP  FACT2N
*21 Heavy Nuclide ------------------------------------------------
U-234     XU040001 922340  232.030     1     2    200.32  0.00   1.0
U-235     XU050001 922350  233.025     3     2    202.25  0.00   1.0
U-236     XU060001 922360  234.018     1     2    202.39  0.00   1.0
U-237     XU070001 922370  235.013     1     0    202.39  0.00   1.0
U-238     XU080001 922380  236.006     2     2    205.92  0.00   1.0
NP237     XNP70001 932370  235.012     1     2    206.05  0.00   1.0
NP239     XNP90001 932390  236.999     1     2    206.05  0.00   1.0
PU238     XPU80001 942380  236.005     1     2    206.05  0.00   1.0
PU239     XPU90001 942390  236.999     3     2    210.96  0.00   1.0
PU240     XPU00001 942400  237.992     2     2    211.01  0.00   1.0
PU241     XPU10001 942410  238.986     3     2    213.27  0.00   1.0
PU242     XPU20001 942420  239.979     1     2    214.29  0.00   1.0
AM241     XAM10001 952410  238.986     1     2    215.25  0.00   1.0
AM242     XAMG0001 952420  239.981     1     0    215.62  0.00   1.0
AM242M    XAMM0001 952421  239.981     1     2    215.62  0.00   1.0
AM243     XAM30001 952430  240.973     1     2    216.00  0.00   1.0
CM242     XCM20001 962420  239.980     1     2    219.48  0.00   1.0
CM243     XCM30001 962430  240.972     1     2    219.86  0.00   1.0
CM244     XCM40001 962440  241.966     1     2    220.25  0.00   1.0
CM245     XCM50001 962450  242.961     1     2    220.63  0.00   1.0
CM246     XCM60001 962460  243.953     1     0    221.02  0.00   1.0
*49 FP + 1 Pseudo Nuclide
KR083     XKR30001 360830   82.287     0     0      0.00  0.00   1.0
ZR095     XZR50001 400950   94.184     0     0      0.00  0.00   1.0
NB095     XNB50001 410950   94.184     0     0      0.00  0.00   1.0
MO095     XMO50001 420950   94.184     0     0      0.00  0.00   1.0
TC099     XTC90001 430990   98.150     0     2      0.00  0.00   1.0
RU101     XRU10001 441010  100.132     0     2      0.00  0.00   1.0
RU103     XRU30001 441030  102.115     0     0      0.00  0.00   1.0
RH103     XRH30001 451030  102.115     0     2      0.00  0.00   1.0
RH105     XRH50001 451050  104.098     0     0      0.00  0.00   1.0
PD105     XPD50001 461050  104.098     0     2      0.00  0.00   1.0
PD107     XPD70001 461070  106.081     0     0      0.00  0.00   1.0
PD108     XPD80001 461080  107.072     0     0      0.00  0.00   1.0
AG107     XAG70001 471070  106.081     0     2      0.00  0.00   1.0
AG109     XAG90001 471090  108.064     0     2      0.00  0.00   1.0
I-135     XI050001 531350  133.840     0     0      0.00  0.00   1.0
XE131     XXE10001 541310  129.875     0     2      0.00  0.00   1.0
XE133     XXE30001 541330  131.857     0     0      0.00  0.00   1.0
XE135     XXE50001 541350  133.840     0     0      0.00  0.00   1.0
          :
          :
GD154     XGD40001 641540  152.677     0     0      0.00  0.00   1.0
GD155     XGD50001 641550  153.668     0     2      0.00  0.00   1.0
```

```
GD156    XGD60001 641560  154.660    0    0     0.00  0.00   1.0
GD157    XGD70001 641570  155.651    0    2     0.00  0.00   1.0
GD158    XGD80001 641580  156.643    0    0     0.00  0.00   1.0
GD160    XGD00001 641600  158.626    0    0     0.00  0.00   1.0
ZZ050    XZ500001   500  114.399    0    0     0.00  0.00   1.0
*** 16 Burnable Poisons ------------------------------------------
B-010    XB000001  50100   9.9269  -10    0     0.00  0.00   1.0
CD113    XCD30001 481130  112.029   -10    0     0.00  0.00   1.0
CD114    XCD40001 481140  113.021   -10    0     0.00  0.00   1.0
IN115    XIN50001 491150  114.012   -10    2     0.00  0.00   1.0
GD152    XGD20001 641520  150.694   -10    0     0.00  0.00   1.0
ER162    XER20001 681620  160.608   -10    0     0.00  0.00   1.0
ER164    XER40001 681640  162.591   -10    0     0.00  0.00   1.0
ER166    XER60001 681660  164.574   -10    2     0.00  0.00   1.0
ER167    XER70001 681670  165.565   -10    2     0.00  0.00   1.0
ER168    XER80001 681680  166.557   -10    2     0.00  0.00   1.0
ER170    XER00001 681700  168.540   -10    2     0.00  0.00   1.0
HF176    XHF60001 721760  174.488   -10    0     0.00  0.00   1.0
HF177    XHF70001 721770  175.479   -10    2     0.00  0.00   1.0
HF178    XHF80001 721780  176.471   -10    2     0.00  0.00   1.0
HF179    XHF90001 721790  177.462   -10    2     0.00  0.00   1.0
HF180    XHF00001 721800  178.454   -10    2     0.00  0.00   1.0
*----------------------------------------------------------------------
*NUCL   NCH   HALFT TUNIT (A8,I2,E10.3,A8) for Block-3-1
U-234    2  2.455E+5YEARS
*NUCLP   NBIC        PBIC (A8,2X,A8,2X,E12.5) for Block-3-2
U-235     2N         1.000
PU238     ALPHA      1.000
* Repeat from Block-3-1 to Block-3-2 NMAX Times
U-235    3  7.038E+8YEARS
U-234     CAPTURE    1.000
U-236     2N         1.000
PU239     ALPHA      1.000
*
U-236    4  2.340E+7YEARS
U-235     CAPTURE    1.000
NP237     2N        0.3744
U-237     2N         1.000
PU240     ALPHA      1.000
*
U-237    3  6.75    DAYS
U-236     CAPTURE    1.000
U-238     2N         1.000
PU241     ALPHA      0.000025
*
U-238    2  4.468E+9YEARS
U-237     CAPTURE    1.000
PU242     ALPHA      1.000
*          :
           :
*
CM246    1   4730.0 YEARS
CM245     CAPTURE    1.0000
*
*Block-3 for Fission Products and Burnable Poisons
KR083    0   0.0    SECONDS
*
ZR095    0  64.02   DAYS
*
NB095    1  34.975  DAYS
ZR095     BETA-      0.999775
*
MO095    2   0.0    SECONDS
ZR095     BETA-      0.000225
NB095     BETA-      1.0000
*
TC099    0 2.1100E+5YEARS
           :
```

```
          :
GD157    2   0.0    SECONDS
EU156     CAPTURE     1.0000
GD156     CAPTURE     1.0000
*
GD158    1   0.0    SECONDS
GD157     CAPTURE     1.0000
*
GD160    0   0.0    SECONDS
*
ZZ050    0   0.0    SECONDS
*
*================== Burnable Poisons (no FP yield data is given)
*
B-010    0   0.0    SECONDS
*
CD113    0 9.300E+15YEARS
*
CD114    1   0.0    SECONDS
CD113     CAPTURE     1.0000
*
IN115    1 4.410E+14YEARS
CD114     CAPTURE     0.966956
*
          :
          :
*
HF180    1   0.0    SECONDS
HF179     CAPTURE     1.0000
*
*Repeat from Block-4-1 to Block-4-3 NYLDTY Times
*FP-Yield-Data for Thermal Fission of U-235
*NAMYLD         NYNUCL    NFP (A8,*) for Block-4-1
YU235T           1       50
*(NAMFIS(I),I=1,NYNUCL) (5(A8,2X)) for Block-4-2
U-235
*NAMFP       YLDFP for Block-4-3, Repeat NFP Times
KR083      5.38052E-03
ZR095      6.49607E-02
NB095      1.26475E-06
MO095      6.03518E-09
TC099      6.11047E-02
          :
          :
GD160      3.16238E-06
ZZ050      1.56236E+00
*FP-Yield-Data for Fast Fission of U-236, U-237
YU236F           3       50
U-234    U-236    U-237
KR083      5.22132E-03
ZR095      6.41135E-02
          :
          :
ZZ050      1.54703E+00
*FP-Yield-Data for Fast Fission of U-238, Pu-238
YU238F           2       50
U-238    PU238
KR083      3.86596E-03
ZR095      5.10681E-02
          :
          :
ZZ050      1.50348E+00
*FP-Yield-Data for Fast Fission of Np-237, Np-239
YNP237F          2       50
NP237    NP239
KR083      4.81007E-03
ZR095      5.69951E-02
          :
```

```
         :
ZZ050      1.50080E+00
*FP-Yield-Data for Thermal Fission of Pu-239
YPU239T          1       50
PU239
KR083      2.94999E-03
ZR095      4.89422E-02
         :
         :
ZZ050      1.45671E+00
*FP-Yield-Data for Fast Fission of Pu-240
YPU240F          1       50
PU240
KR083      3.02678E-03
ZR095      4.39651E-02
         :
         :
ZZ050      1.44366E+00
*FP-Yield-Data for Thermal Fission of Pu-241,Am-242g,m,Cm-243,Cm-245
YPU241T          5       50
PU241    AM242    AM242M   CM243    CM245
KR083      2.11888E-03
ZR095      4.07446E-02
         :
         :
ZZ050      1.41174E+00
*FP-Yield-Data for Fast Fission of Pu-242,Am-241,Am-243,Cm242,Cm244,Cm246
YPU242F          6       47
PU242    AM241    AM243    CM242    CM244
CM246
KR083      2.39524E-03
ZR095      4.02262E-02
         :
         :
GD160      4.59798E-04
ZZ050      1.41556E+00
**********************
```

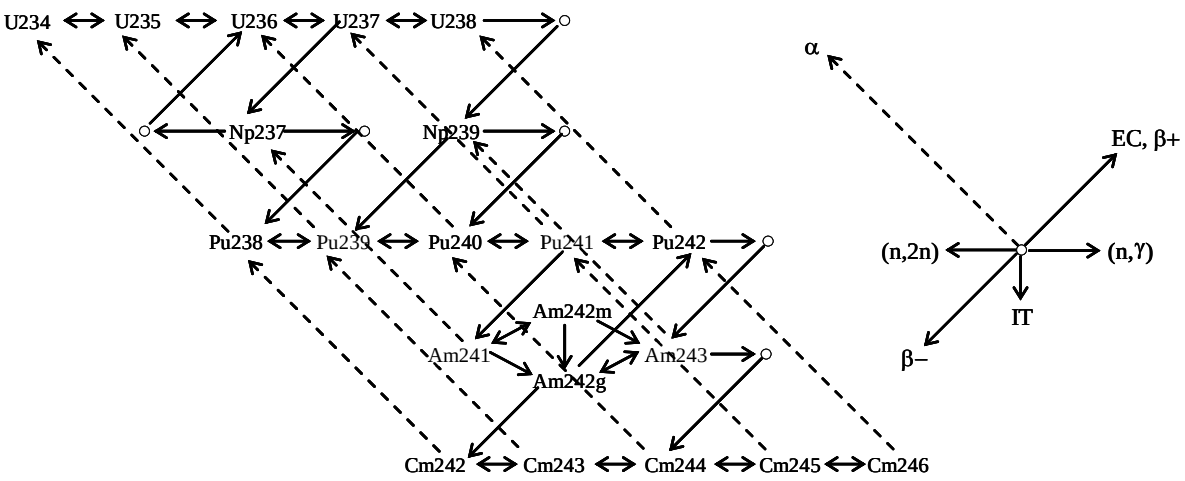


Fig. 3.3-1 Burn-up chain model for heavy nuclides (models : u4cm6~)

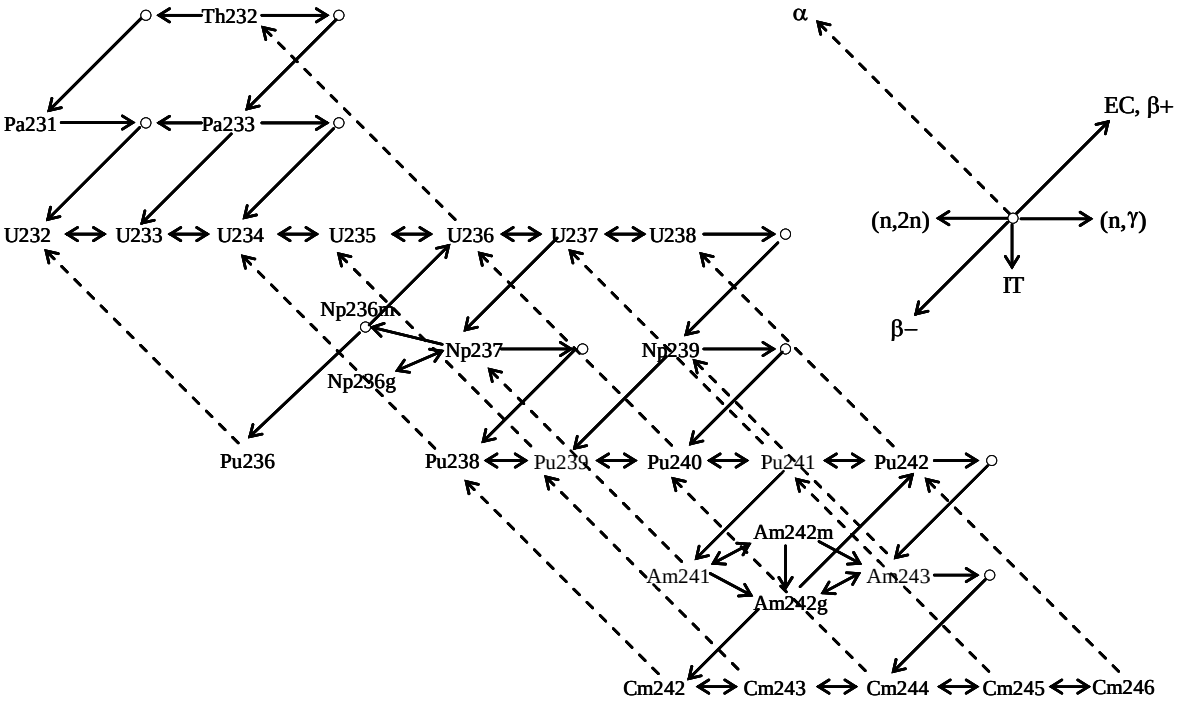


Fig. 3.3-2 Burn-up chain model for heavy nuclides (models : th2cm6~)

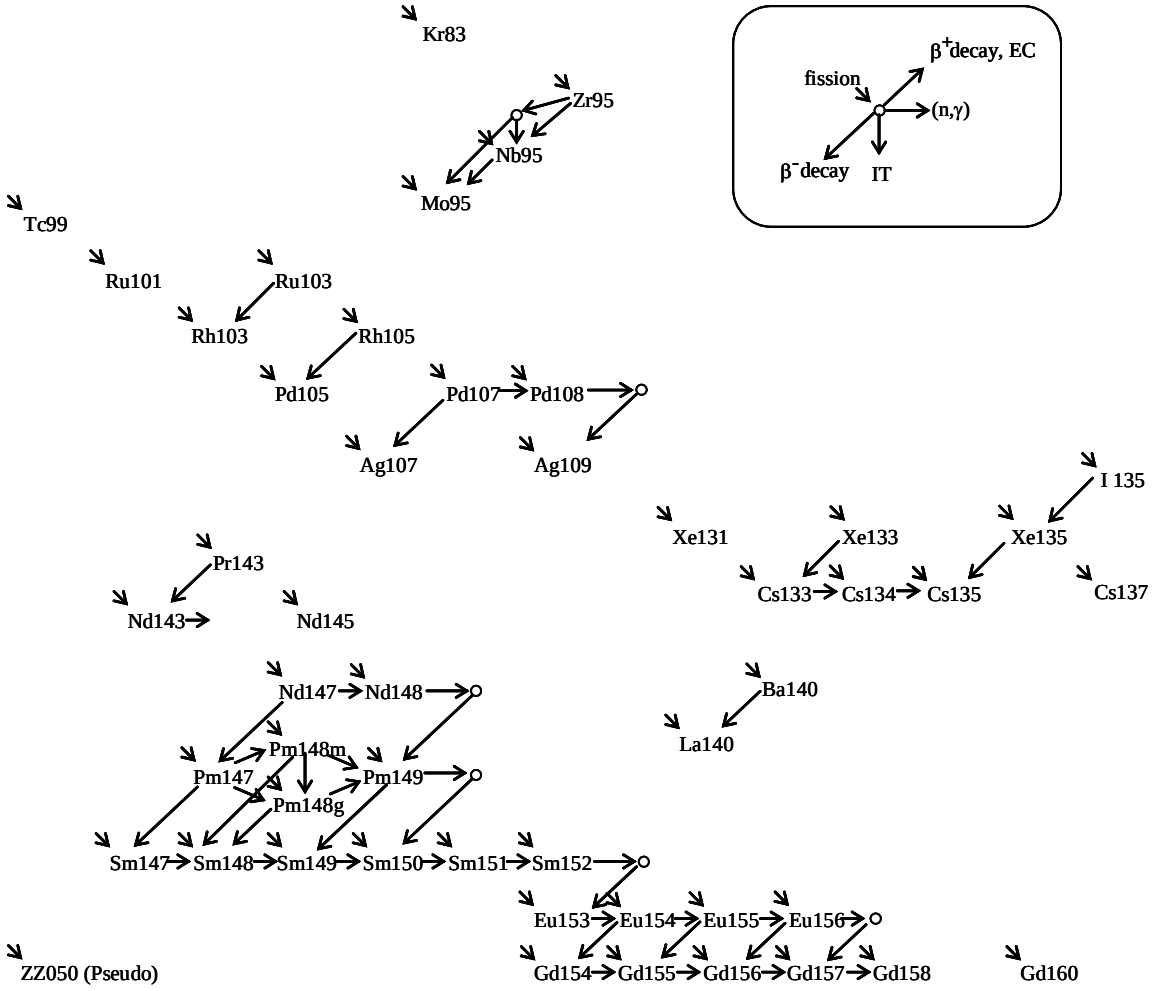


Fig. 3.3-3 Burn-up chain model for fission products and burnable poisons (models : ~fp50bp16T/F)

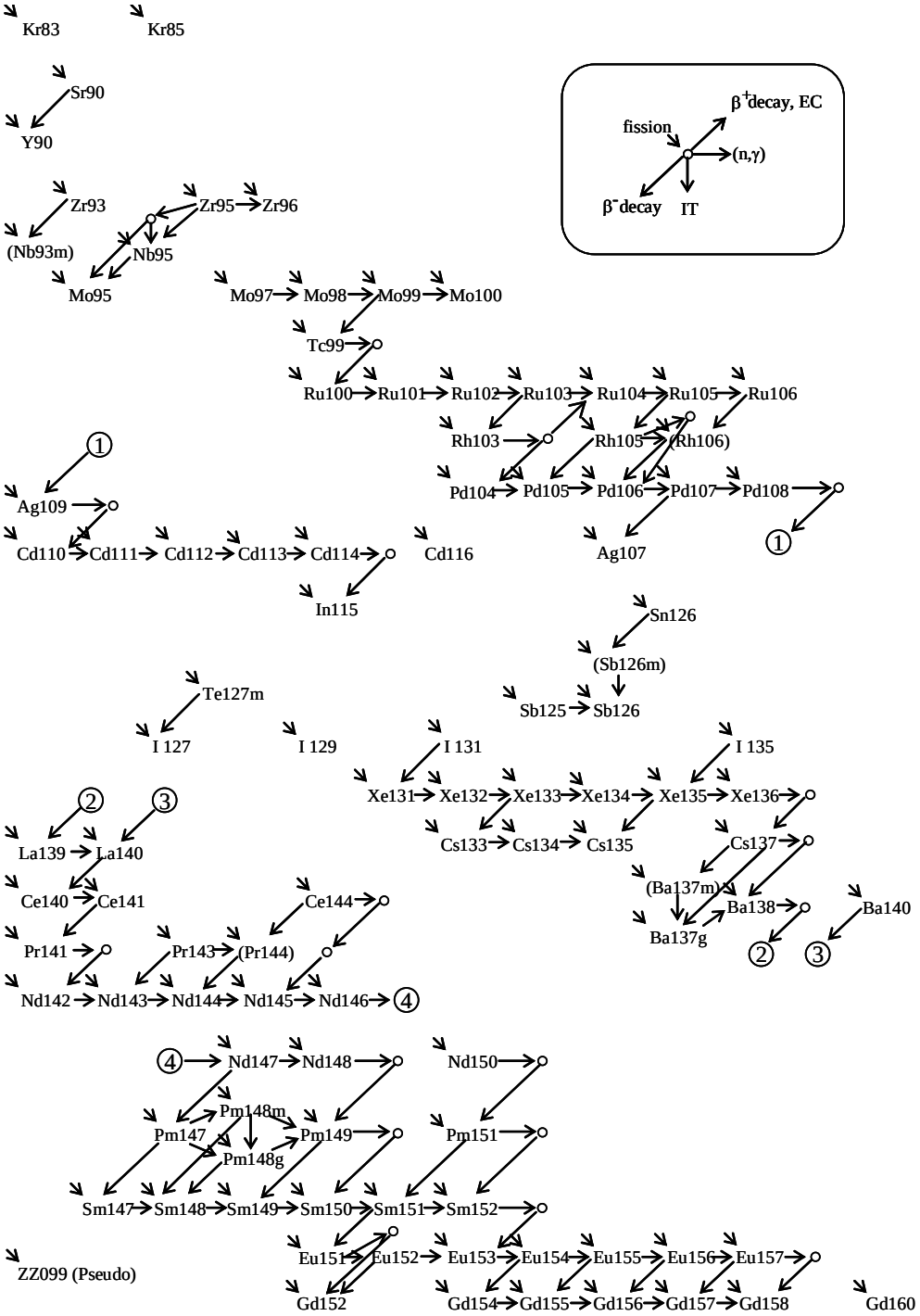


Fig. 3.3-4 Burn-up chain model for fission products and burnable poisons (models: ~fp104bp12T/F)

Note: Nuclides in parentheses have no cross-section data, only time-decay is considered.

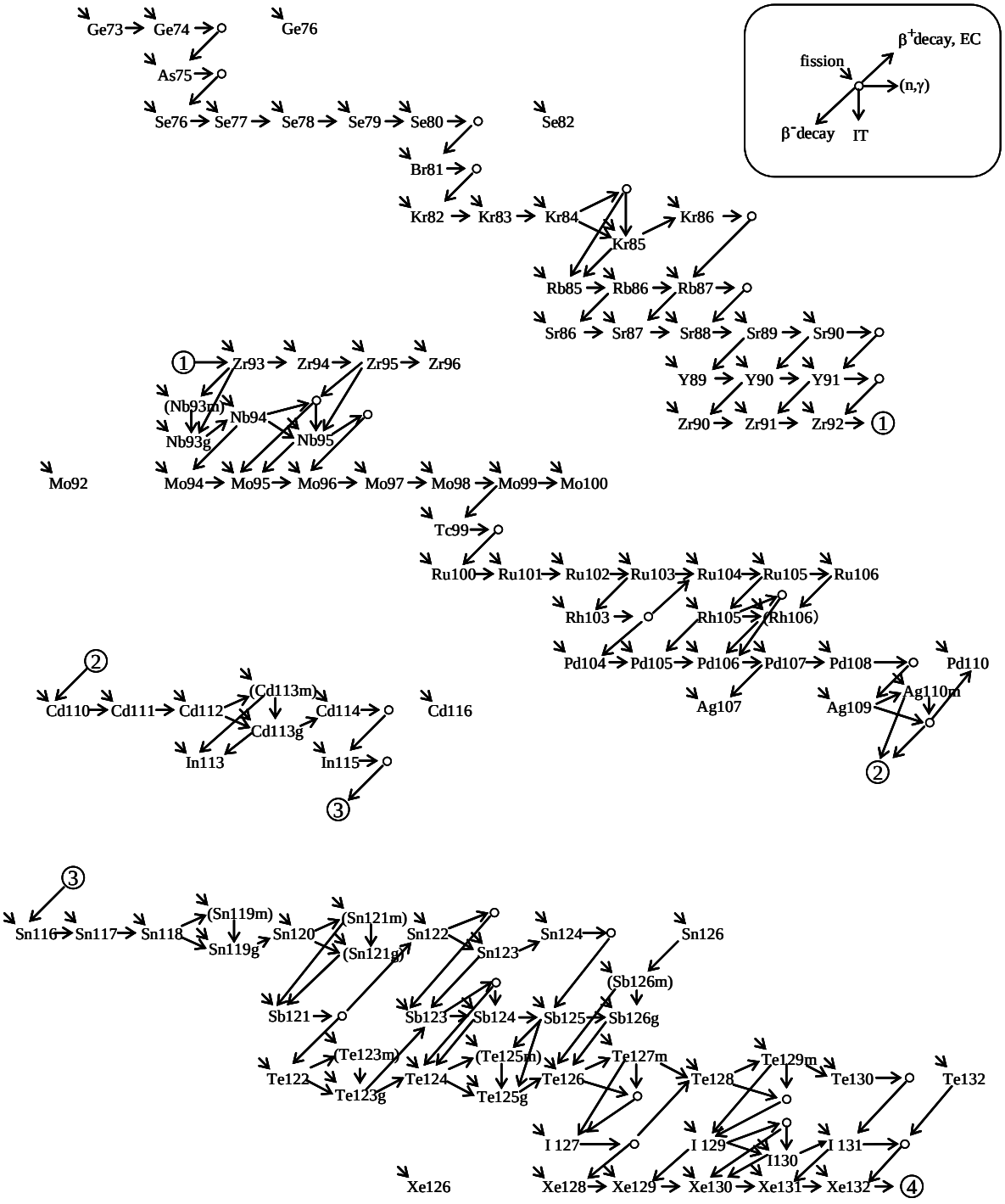


Fig. 3.3-5 (1/2) Burn-up chain model for fission products and burnable poisons (models: ~fp193bp6T/F)

Note: Nuclides in parentheses have no cross-section data, only time-decay is considered.

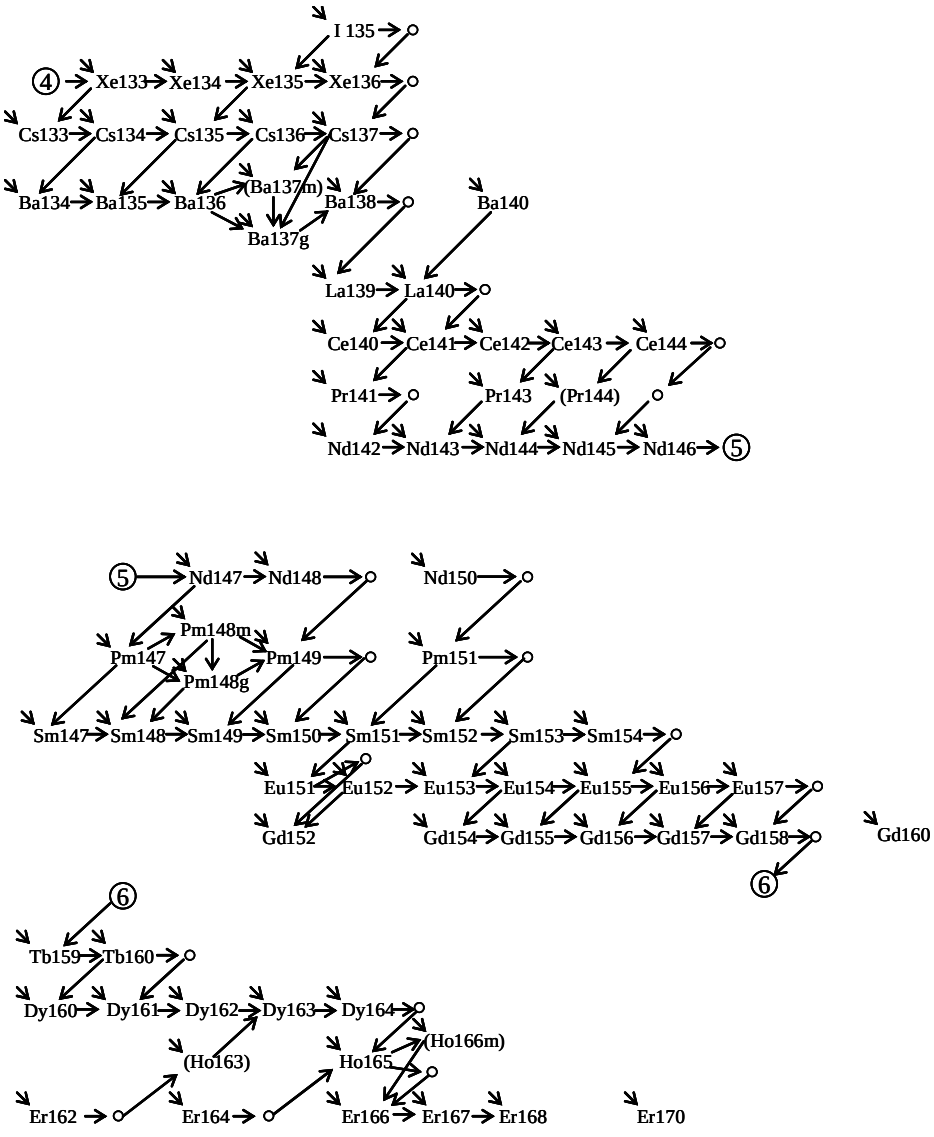


Fig. 3.3-5 (2/2) Burn-up chain model for fission products and burnable poisons (models: ~fp193bp6T/F)

4. Job Control Statements

In this chapter, job control statements will be described by C-shell-script for the machine that works on the UNIX operating system. A typical sample shell-script is shown below. In this sample, it is assumed that the user's home directory ($Home) is '/home/okumura' and the SRAC system is installed in the directory '/home/Administrator'.

```
#!/bin/csh
#-----------------------------------------------------
#  <<  Sample shell script for SRAC execution  >>
#
#
#       At least, lines in bold face shoud be changed by each user
#
#
#-----------------------------------------------------
#
#============= to use native UNIX command
   alias   mkdir  mkdir
   alias   cat    cat
   alias   cd     cd                  ..................................(a)
   alias   rm     rm
#
#============= Set by user
#
#  LMN    : name of a load module in ~SRAC/bin/
#  BRN    : burnup chain data file in ~SRAC/lib/burnlibT/
#           =u4cm6fp50bp16T  : (standard model for thermal reactors)
#  ODR    : directory for output of text files
#  CASE   : arbitrary case name for output files
#  WKDR   : work directory for SRAC execution
#  PDSD   : directory for PDS files
#
   set SRAC_DIR = /home/Administrator/SRAC ..............................(b)
   set LMN      = SRAC.100m .............................................(c)
   set BRN      = u4cm6fp50bp16T ........................................(d)
   set ODR      = $HOME/Job/MyOutput ....................................(e)
   set CASE     = Test-1 ................................................(f)
   set PDSD     = $HOME/Job/Mypds .......................................(g)
#
#=============  mkdir for PDS
#
#  PDS_DIR : directory name of PDS files
#  PDS file names must be identical to those in input data
#
   set PDS_DIR = $PDSD/$CASE
   mkdir $PDS_DIR
   mkdir $PDS_DIR/UFAST
   mkdir $PDS_DIR/UTHERMAL
   mkdir $PDS_DIR/UMCROSS              ..................................(h)
   mkdir $PDS_DIR/MACROWRK
   mkdir $PDS_DIR/MACRO
   mkdir $PDS_DIR/FLUX
   mkdir $PDS_DIR/MICREF
#
#=============  Change if necessary
   set LM       = $SRAC_DIR/bin/$LMN ....................................(i)
   set DATE     = `date +%b%d.%H.%M.%S` .................................(j)
   set WKDR     = $HOME/SRACtmp.$CASE.$DATE .............................(k)
   mkdir $WKDR
#
```

```
   setenv  fu50  $SRAC_DIR/lib/burnlibT/$BRN ..............................(l)
   setenv  fu85  $SRAC_DIR/lib/kintab.dat ..................................(m)
#  setenv  fu89  $ODR/$CASE.SFT89.$DATE ....................................(n)
#  setenv  fu98  $ODR/$CASE.SFT98.$DATE ....................................(o)
   setenv  fu99  $ODR/$CASE.SFT99.$DATE ....................................(p)
   set OUTLST =  $ODR/$CASE.SFT06.$DATE.....................................(q)
#
#=============  Exec SRAC code with the following input data =============
#
cd $WKDR
cat - << END_DATA | $LM >& $OUTLST ......................................(r)
TEST
SRAC INPUT for Cell Calculation by Pij                          Input Data
1 1 1 1 0   1 4 3 -2 1   0 0 0 0 2   0 1 0 0 0 / SRAC CONTROL
2.77396E-4  / GEOMETRICAL BUCKLING
/home/Administrator/SRACLIB-JDL33/pds/pfast   Old   File
/home/Administrator/SRACLIB-JDL33/pds/pthml   O     F      ..........(s)
/home/Administrator/SRACLIB-JDL33/pds/pmcrs   O     F
$PDS_DIR/UFAST         Scratch Core
$PDS_DIR/UTHERMAL      S       C
$PDS_DIR/UMCROSS       S       C
$PDS_DIR/MACROWRK      S       C      ..............................(t)
$PDS_DIR/MACRO         New     C
$PDS_DIR/FLUX          S       C
$PDS_DIR/MICREF        S       C
62 45  2 1   /  107 group => 3 group
62(1)        /
          :
          :
          :
END_DATA ................................................................(u)
#
#========  Remove scratch PS files ========================================
#
   cd $HOME
   rm -r $WKDR ..........................................................(v)
#
#========  Remove PDS files if you don't keep them ========================
#
#  rm -r $PDS_DIR
#
  rm -r $PDS_DIR/UFAST
  rm -r $PDS_DIR/UTHERMAL
  rm -r $PDS_DIR/UMCROSS      ..................................(w)
  rm -r $PDS_DIR/MACROWRK
#  rm -r $PDS_DIR/MACRO
  rm -r $PDS_DIR/FLUX
  rm -r $PDS_DIR/MICREF
```

Underlined statements below indicate actions by user when he uses the above shell-script.

(a) In the shell-script, several native UNIX commands are used, however, the user may customize their operations. By using ‘alias’ command, it is recovered to native ones during this process.

(b) Specify the SRAC system by full path directory name.

(c) Specify the SRAC load module (executable) in the directory file ~SRAC/bin/.

A load module, ‘SRAC.100m’ by name is usually installed by the equipped installer (@PunchMe). This load module is made to be executable on the memory within about 100Mbyte. For a large-scale problem, another load may be necessary. It can be made by using a shell-script,

~SRAC/tool/lmmake/lmmk/lmmk.sh, which is made by the installer.

(d) Specify an appropriate burn-up chain library data that is used in burn-up calculation. [cf. Sect. 3.3]. Available burn-up chain data files (text data) are stored in ~SRAC/lib/burnlibT/.

(e) All useful output files except PDS is stored in the directory specified here.

(f) Give arbitrary case name for current calculation process. This case name has no relation to the case name specified in SRAC input data 'CASENAME' in Sect.2.2. The case name here is used to name output files, PDS files, and work directories described below [(h), (j), (n)~(q)]. Therefore, too long name or name including inappropriate characters as file name should be avoided.

(g) Specify an existing user's directory, in which PDS files are created.

(h) Empty PDS files (=directories) are made here. In this sample, full path directory name of MACRO file is '/home/okumura/Job/Mypds/Test-1/MACRO'.

(i) A load module of SRAC is specified here by full path name. In this sample, it is: '/home/Administrator/SRAC/bin/SRAC.100m'.

(j) The Unix command 'date' with format parameters gives current date and time as 'Dec25.11.22.33' (11h. 22m. 33s. on Christmas). This expression may be different by environment of user's system. The expression is connected to name of output file. If it is inappropriate on the system or dislikable, change it.

(k) The SRAC code is executed in the directory specified here. In this case, it is: '/home/okumura/SRACtmp.Test-1.Dec25.11.22.33'
Don't remove this directory during SRAC executing. Some scratch files may be made in it.

(l) The burn-up chain data specified in (d) is allocated to the 50th device.

(m) The file 'kintab.dat' is a binary data including the Bickley function table used by PIJ, which is made by the installer @PunchMe.

(n) Set this line active (erase # in the first column), if plot option is used by PIJ or PEACO (cf. Sec.1.11, Sect.2.4 and 2.12). Plot data is stored on the 89th file. It is portable among machines, because it is a normal text file (PostScript file).

(o) Set this line active, when option for burn-up calculation is used (IC20=1 in Sect.2.2), and if summary table of burn-up calculation results is necessary.

(p) Major calculated results are printed on the file of 99th device, but not on the standard output file. Name of the file in this case is: '/home/okumura/Job/Myoutput/Test-1.SFT99. Dec25.11.22.33'.

(q) The name of the standard output file is set here as same as above (not SFT99 but SFT06). Information on progress of calculation and/or error messages are printed on this file. The user may browse it during SRAC execution but he must not edit and save it.

(r) The UNIX command 'cat' has a function to display files. Here, it is used to give the load module a standard input data of SRAC starting from next line to the line before 'END_DATA' [See (u)].

Pay attention that the letters starting from '$' is taken as an environmental variable even if it appears in the input data field. [See (t)]. The character '$' must not be used, for instance, in comment line of SRAC input. As usual, an input data file can be separately specified by:

$LM < [input file] >& $OUTPUT

(s) Specify the Public Libraries to be used.

(t) Specify the Users PDS files in the standard input data. It is convenient to use the environmental variable, which is expanded at the execution step. It should be noted that allowed input data field is up to 72 columns. The user must consider the length of input record when the variable is expanded.

So called symbolic linking by the UNIX command '*ln*' is useful to make long path name shorter:

e.g. ' ln -s [real-file] [alias-file] '

(u) 'END_DATA' indicates end of the standard input data described before.

(v) Work directory is removed after the completion of SRAC calculation.

(w) Many member files are stored in User's PDS files. Remove them if they are not necessary. In this case, only MACRO file is preserved. If 'Scratch' is specified for a PDS at the SRAC input [See (t)], all member files in the PDS are automatically removed by code, although an empty directory file is left.

5. Sample Input

Several typical examples for SRAC will be shown in this chapter. Input data files for the examples are stored in a directory: ~SRAC/smpl/shr/.

5.1 Cell Burn-up Calculation (PIJ)

A sample input of a cell burn-up calculation for a pin cell model of a PWR (Fig.5.1-1) is shown below, where cell calculation by PIJ is executed on 107-group structure (fast 62, thermal 45 groups) with PEACO option for effective resonance cross-sections. It is assumed that the fuel pin is exposed until 31.4GWd/t with the local power history shown in Fig. 5.1-2. At each burn-up step, neutron multiplication factor and fuel composition are evaluated and two group collapsed constants are preserved on MACRO file. This calculation is based on the post irradiation analysis for the spent fuel from Japanese PWR (Mihama-3) [30), 31)].

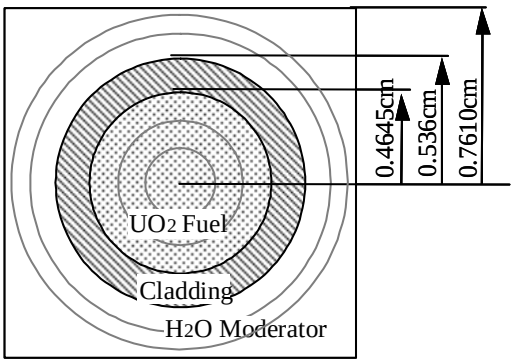


Fig.5.1-1 Cell geometry of the sample input for cell burn-up calculation

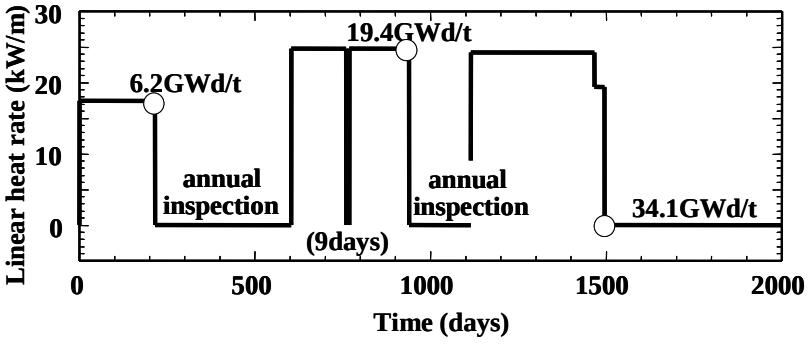


Fig.5.1-2 Power history of irradiated UO_2 fuel sample in PWR (Mihama-3 PIE)

[File name: PIE.sh]----------

```
NO08
PIE analysis of Mihama-3 Sample 87C08 : JAERI-M 93-061 pp162
1 1 1 1 2   1 4 3 -2 1   0 0 0 0 1   2 1 0 0 1 / SRAC CONTROL
1.000E-20 / Geometrical buckling for P1/B1 calculation
*- PDS files ------2---------3---------4---------5---------6---------7--
* Note : All input line must be written in 72 columns except comments
*       even when environmental variables are expanded.
*--------1---------2---------3---------4---------5---------6---------7--
/home/okumura/SRACLIB-JDL33/pds/pfast   Old     File
/home/okumura/SRACLIB-JDL33/pds/pthml   O       F
/home/okumura/SRACLIB-JDL33/pds/pmcrs   O       F
/home/okumura/Mypds/PIE/UFAST           Scratch Core
/home/okumura/Mypds/PIE/UTHERMAL        S       C
/home/okumura/Mypds/PIE/UMCROSS         S       C
/home/okumura/Mypds/PIE/MACROWRK        S       C
/home/okumura/Mypds/PIE/MACRO           S       C
/home/okumura/Mypds/PIE/FLUX            S       C
/home/okumura/Mypds/PIE/MICREF          S       C
************************************************************************
62 45  1 1 /  107 group => 2 group
62(1)     /  Energy group structure suggested for LWR analyses
45(1)     /
62       / Fast    1 group
45       / Thermal 1 group
***** Enter one blank line after input for energy group structure

***** Input for PIJ (Collision Probability Method)
4 7 7 3 1   1 7 0 0 0   5 0 6 15 0   0 45 0        / Pij Control
0 50 50 5 5 5 -1  0.0001 0.00001 0.001 1.0 10. 0.5  /
1 1 1 2 3 3 3 /  R-S
3(1)          /  X-R
1 2 3         /  M-R
* effective cell pitch to presearve a spectrum index at sample fuel
0.0  0.2682 0.3793 0.4645   0.536   0.611 0.686 0.7610  / RX
****** Input for material specification
3 / NMAT
FUE1X01X  0 5 1150.  0.929   0.0  / 1 : UO2 fuel (3.25a/o)
XU040000  2 0  6.8257E-6      /1
XU050000  2 0  7.3957E-4      /2
XU080000  2 0  2.2005E-2      /3
XU060000  2 0  7.5020E-6      /4
XO060000  0 0  4.5518E-2      /5
CLD1X02X  0 3  608.  0.142   0.0  / 2 : cladding
XZRN0000  0 0  4.2982E-2      /1
XFEN0000  0 0  1.4838E-4      /2
XCRN0000  0 0  7.5891E-5      /3
MOD1X03X  0 4  588.  1.0    0.0  / 3 : moderator
XH01H000  0 0  4.6368E-2      /1  Density at 588K = 0.6936 g/cc
XO060000  0 0  2.3184E-2      /2
XB000000  0 0  3.7885E-6      /3
XB010000  0 0  1.5541E-5      /4
****** Input for cell burn-up calculation
20 3 1 1 0  0 0 0 0 1  10(0)   / IBC : burnup control
* Power history is normalized to achieve exporsure of sample fuel : 34.1GWd/t
3(1.73488e-04)    &
  0.00000e+00     & cooling
3(2.45971e-04)
  0.00000e+00     & cooling
4(2.45971e-04)
  0.00000e+00     & cooling
4(2.40521e-04)
2(1.92866e-04)
  0.00000e+00     / Power (MW/cm)
* Exposure in unit : accumulated days
10.0 100.0 215.0  &
603.0           & cooling
```

```
613.0 650.0 760.0
769.0          & cooling
780.0 850.0 900.0 939.0
1115.0         & cooling
1125.0 1200.0 1300.0 1467.0
1480.0 1495.0
3320.0         & cooling (5 years after irradiation)
* optional input for IBC10 (specification of burnable materials)
1 0 0   / Boron in water is not depleted
****** Input for PEACO option
0   / no plot
```
one blank line (null case name to terminate job)

Major part of output list is shown below.

```
<<<< RESULT-OF-DEPLETION-CALCULATION >>>>
 CASEID=NO08
 TITLE: PIE analysis of Mihama-3 Sample 87C08 : JAERI-M 93-061 pp162
 :
 :
 * DAYS        0.00000e+00 1.00000e+01 1.00000e+02 2.15000e+02 6.03000e+02
 * MWD/TON     0.00000e+00 2.84616e+02 2.84616e+03 6.11925e+03 6.11925e+03
 * U05-%       0.00000e+00 1.05201e+00 9.95800e+00 2.01382e+01 2.01379e+01

 * K-EFF       1.278347   1.233094   1.203718   1.165625   1.196787
 * K-INF       1.278347   1.233094   1.203718   1.165625   1.196787

 * INST.-C.R.  0.449554   0.461295   0.470528   0.497071   0.486592
 * INTE.-C.R.  0.449554   0.460112   0.465757   0.465757   0.467091
 * MWD         0.00000e+00 1.73488e-03 1.73488e-02 3.72999e-02 3.72999e-02
 * POWER(MW)   1.73488e-04 1.73488e-04 1.73488e-04 0.00000e+00 2.45971e-04
 * TON-HM      6.09551e-06 6.09371e-06 6.07758e-06 6.05703e-06 6.05703e-06
 * FLUX-LEVEL  2.02809e+14 2.09282e+14 2.15129e+14 0.00000e+00 3.09189e+14
 * FIS.-ABSOR  6.14700e+12 6.15440e+12 6.28730e+12 5.53339e-01 9.08457e+12
 * FIS.-DECAY  0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
 * FER.-CAPTR  2.76341e+12 2.83899e+12 2.95835e+12 2.75049e-01 4.42048e+12


MATERIAL-NO.=  1   VOLUME= 6.77830e-01 (CC)   WEIGHT= 8.99268e-06 (TON/CC)


 * DAYS        0.00000e+00 1.00000e+01 1.00000e+02 2.15000e+02 6.03000e+02
 * MWD/TON     0.00000e+00 2.84616e+02 2.84616e+03 6.11925e+03 6.11925e+03
 * POW(MW/CC)  2.55946e-04 2.55946e-04 2.55946e-04 0.00000e+00 3.62880e-04
 * ENRGY/FIS.  3.24372e-11 3.24498e-11 3.25767e-11 3.27006e-11 3.27029e-11
 * XE-135-YD.  2.29916e-03 2.36834e-03 3.17121e-03 3.90081e-03 3.92924e-03
 *  I-135-YD.  6.31723e-02 6.31955e-02 6.33534e-02 6.35348e-02 6.35285e-02
 * SM-149-YD.  1.04750e-10 1.25311e-10 3.53129e-10 5.60200e-10 5.67467e-10
 * PM-149-YD.  1.09672e-02 1.09929e-02 1.11644e-02 1.13452e-02 1.13395e-02
 ---- -------- ----------- ----------- ----------- ----------- -----------
    1 U-234    6.82570e-06 6.79931e-06 6.56349e-06 6.26847e-06 6.26887e-06
    2 U-235    7.39570e-04 7.31790e-04 6.65924e-04 5.90634e-04 5.90636e-04
    3 U-236    7.50200e-06 8.88524e-06 2.05732e-05 3.37919e-05 3.37925e-05
    4 U-237    0.00000e+00 1.66895e-08 4.23827e-08 6.31501e-08 5.42947e-14
    5 U-238    2.20050e-02 2.20011e-02 2.19653e-02 2.19181e-02 2.19181e-02
    6 NP237    0.00000e+00 9.82919e-09 3.08541e-07 8.95561e-07 9.58811e-07
    7 NP239    0.00000e+00 1.13531e-06 1.21175e-06 1.25603e-06 1.78496e-15
     :
     :
```

5.2 Reaction Rate Calculation (PIJ)

Figure 5.2-1 shows a hexagonal array of two different fuel rods in the PROTEUS-LWHCR (CORE-6) experiment[32] simulating a high-conversion light water reactor. Below is a sample input to evaluate nuclide-wise reaction rate in two different fuels by using the neutron fluxes obtained by cell calculation with 107 group structure. The output reaction rates by this sample are fission and capture rates at energy ranges fast (1st to 67th), thermal (68th to 107th) and the whole (1st to 107th) for the nuclides U-235, Pu-239, Pu-240, Pu-241, Am-241, U-233 and Th-232.

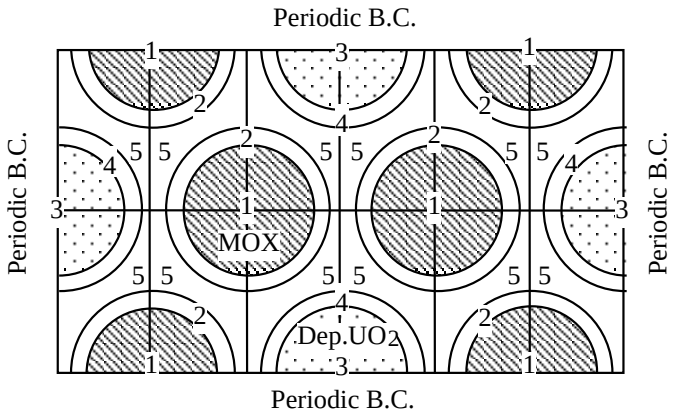


Fig.5.2-1 Cell geometry of a sample input for reaction rate calculation

[File name: React.sh]----------

```
COR6
PROTEUS-LWHCR Experiment (Core 6, 0% Void)
1 1 1 1 2   1 4 3 -12 1   0 0 0 0 1   2 1 1 0 0 / SRAC Control
2.0507E-3  / Buckling (Critical searced value)
*- PDS files ------2---------3---------4---------5---------6---------7--
/home/okumura/SRACLIB-JDL33/pds/pfast      Old           File
/home/okumura/SRACLIB-JDL33/pds/pthml      O             F
/home/okumura/SRACLIB-JDL33/pds/pmcrs      O             F
/home/okumura/Mypds/React/UFAST            Scratch       Core
/home/okumura/Mypds/React/UTHERMAL         S             C
/home/okumura/Mypds/React/UMCROSS          S             C
/home/okumura/Mypds/React/MACROWRK         S             C
/home/okumura/Mypds/React/MACRO            S             C
/home/okumura/Mypds/React/FLUX             S             C
/home/okumura/Mypds/React/MICREF           S             C
62 45  1 1     /  107 group => 2 group
62(1)          /  Energy group structure suggested for LWR analyses
45(1)          /
62             / Fast    1 group
45             / Thermal 1 group
***** Enter one blank line after input for energy group structure

***** Input for PIJ (Collision Probability Method)
13 32 5 5 1   1 6 2 10 0   3 0 10 29 2   1 180 1          / Pij Control
0 20 50 5 5 5 -1  0.0001 0.00001 0.001 1.0 10. 0.5       /
```

```
  5  5  5  5  5  5      &
  5  5  5  5  5  5      &
   1 2  3 4  1 2       &
 3 4  1 2  1 2  3 4    &
   1 2  3 4  1 2       &  T-S
5(1)                   /  X-R
1 2 3 4 5              /  M-R
0.0  6*0.45            /  RX
0.0  2*0.77942          /  TY
2 4 6   1 3 5 7  2 4 6    /  IXP
1 1 1   2 2 2 2  3 3 3    /  IYP
10( 0.0  0.335  0.411 )   /  RDP
12 1 1                  /  Plot Pij Geometry
****** Input for material specification
5 / NMAT
MAT1X01X  0 18 300. 0.67  0.58755  /  MAT  1 : FUEL ROD(15% PU2/UO2)
XU050001  2 0 7.781E-05  / 1
XU080001  2 0 1.839E-02  / 2
XPU90001  2 0 2.580E-03  / 3
XPU00001  2 0 5.699E-04  / 4
XPU10001  2 0 5.675E-05  / 5
XPU20001  2 0 1.256E-05  / 6
XAM10001  2 0 3.833E-05  / 7
XU030001  2 0 1.0E-12    / 8 DUMMY for Reaction Rate Calculation
XTH20001  2 0 1.0E-12    / 9 DUMMY
XO060001  0 0 4.346E-02  /10
XH010001  0 0 2.005E-04  /11
XAL70001  0 0 3.683E-04  /12
XFEN0001  0 0 2.600E-03  /13
XCRN0001  0 0 6.843E-04  /14
XNIN0001  0 0 3.301E-04  /15
XMN50001  0 0 5.376E-05  /16
XSIN0001  0 0 3.286E-05  /17
XMON0001  0 0 8.123E-06  /18
MAT2X02X  0 8 300. 0.10   1.0     /  MAT  2 : CLADDING (STEEL+AIR+AL)
XAL70001  0 0 6.080E-03  / 1
XFEN0001  0 0 3.125E-02  / 2
XCRN0001  0 0 8.536E-03  / 3
XNIN0001  0 0 5.118E-03  / 4
XMN50001  0 0 1.001E-03  / 5
XMON0001  0 0 7.354E-04  / 6
XSIN0001  0 0 8.124E-04  / 7
XN040001  0 0 1.323E-05  / 8
MAT3X03X  0 11 300. 0.67  0.58755  /  MAT  3 : DEPLETED UO2
XU050001  2 0 9.851E-05  / 1
XU080001  2 0 2.328E-02  / 2
XPU90001  2 0 1.0E-12    / 3 DUMMY
XPU00001  2 0 1.0E-12    / 4 DUMMY
XPU10001  2 0 1.0E-12    / 5 DUMMY
XPU20001  2 0 1.0E-12    / 6 DUMMY
XAM10001  2 0 1.0E-12    / 7 DUMMY
XU030001  2 0 1.0E-12    / 8 DUMMY
XTH20001  2 0 1.0E-12    / 9 DUMMY
XO060001  0 0 4.677E-02  /10
XAL70001  0 0 3.827E-04  /11
MAT4X04X  0 8 300. 0.10   1.0     /  MAT  4 : CLADDING (STEEL+AIR+AL)
XAL70001  0 0 6.080E-03  / 1
XFEN0001  0 0 3.125E-02  / 2
XCRN0001  0 0 8.536E-03  / 3
XNIN0001  0 0 5.118E-03  / 4
XMN50001  0 0 1.001E-03  / 5
XMON0001  0 0 7.354E-04  / 6
XSIN0001  0 0 8.124E-04  / 7
XN040001  0 0 1.323E-05  / 8
MAT5X05X  0 2 300. 0.10   1.0     /  MAT  5 : LIGHT WATER (300 D K)
XH01H001  0 0 6.652E-02  / 1
XO060001  0 0 3.326E-02  / 2
****** Input for Reaction rate calculation
```

```
* thermal cut-off energy = 0.99312eV
0 0 10 0  / IOPT(1:4)--------- << Reaction Rate >> -------------------+
1 1 2 1 0 0 67(1.0) 40(0.0) / MPOSI,LU235,LU238,IX,IY,IZ,FGS(1:IGMAX) !
1 3 4 1 0 0 67(1.0) 40(0.0) /                                        !
1 5 6 1 0 0 67(1.0) 40(0.0) /                                        !
1 7 8 1 0 0 67(1.0) 40(0.0) /                                        !
1 9 9 1 0 0 67(1.0) 40(0.0) /                                        !
3 1 2 3 0 0 67(1.0) 40(0.0) /                                        !
3 3 4 3 0 0 67(1.0) 40(0.0) /                                        !
3 5 6 3 0 0 67(1.0) 40(0.0) /                                        !
3 7 8 3 0 0 67(1.0) 40(0.0) /                                        !
3 9 9 3 0 0 67(1.0) 40(0.0) / ---------------------------------------+
0 / PEACO PLOT
```

one blank line (null case name to terminate job)

5.3 S_N Transport Calculation (PIJ, ANISN, TWOTRAN)

The left side figure in Fig.5.3-1 shows a criticality problem of a fuel solution in a cylindrical stainless-steel container of 0.3cm bottom and side wall thickness, 15cm outer radius and 54.249cm total height. This problem is solved by using both of ANISN and TWOTRAN. The calculation scheme consists of the following three cases.

(1) Production of effective cross-sections by PIJ (case name: **`CELL`**)

A fixed source problem is solved for a one-dimensional infinitely long cylindrical system of fuel solution and the container by using PIJ module with 107-group structure. The fine group effective cross-sections are obtained as the result. This case is for the effective resonance calculation by the PEACO option. If the NR or IR approximation is used, this case is not necessary.

(2) Production of few group cross-sections by ANISN (case name: **`ANIS`**)

An eigenvalue is solved for the same geometry as that of the first case (the one-dimensional infinitely long cylindrical system of fuel solution and the container with 107-group structure) by using ANISN one-dimensional Sn module with $P_1 S_8$. In this calculation, the cross-sections are provided by the first case. The axial leakage is taken into accounted by the transverse buckling. The cross-sections are collapsed by the flux obtained by ANISN into 18-group structure. To consider the difference of spectrum of outer part near the vacuum boundary and that of inner part, the cross-sections of fuel solution corresponding to these parts are separately obtained by specifying two homogenization regions (X-Region).

(3) Few group eigenvalue calculation by TWOPTRAN (case name: **`TWOC`**)

The final eigenvalue problem is solved for the R-Z geometry by TWOTRAN: two-dimensional SN module with P_1 S_8 approximation. The 18 group P_0 and P_1 cross-sections for three materials (inner fuel solution, outer one and SS container) are provided by the previous case. The right side figure in Fig.5.3-1 shows material and zone allocation for TWOTRAN.

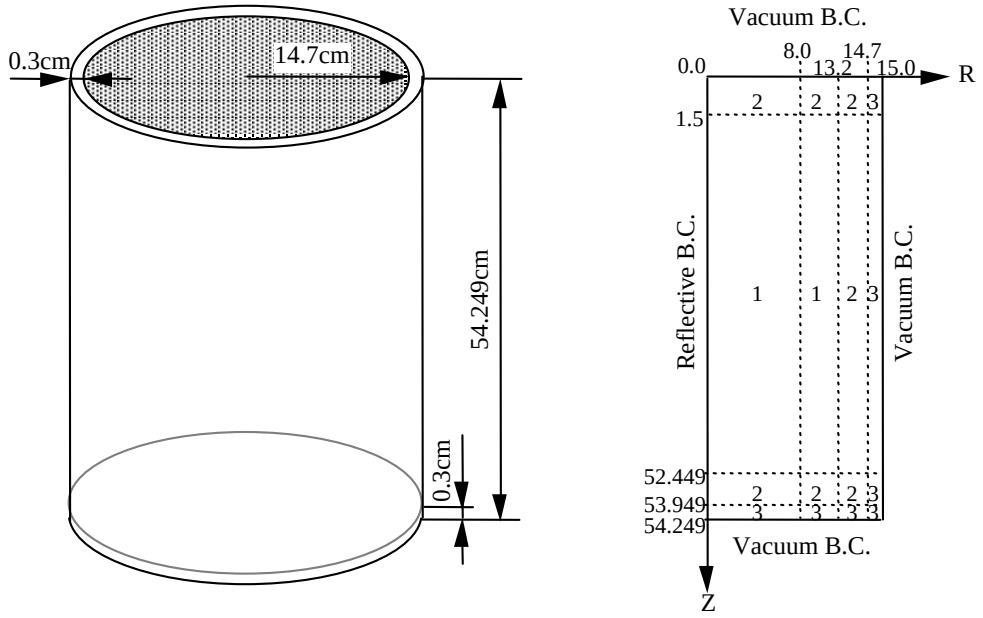


Fig.5.3-1 Core geometry (left) and calculation model by TWORAN (right) of a sample input for S_N transport calculation

[File name: SnSmpl.sh]----------

```
CELL
CRAC:  60.0 G/L : TEMP 40 C : HNO3 1 NOL : 53.52 CM HIGHT : DOPPLER 1
1 1 1 1 2   1 4 3 -2 0   0 0 1 0 2   1 1 0 0 0 / SRAC CONTROL
2.37826E-02 / R"=  16.700 CM  H"=  56.949 CM
/home/okumura/SRACLIB-JDL33/pds/pfast      Old           File
/home/okumura/SRACLIB-JDL33/pds/pthml      O             F
/home/okumura/SRACLIB-JDL33/pds/pmcrs      O             F
/home/okumura/Mypds/SnSmpl/UFAST           Scratch       Core
/home/okumura/Mypds/SnSmpl/UTHERMAL        S             C
/home/okumura/Mypds/SnSmpl/UMCROSS         S             C
/home/okumura/Mypds/SnSmpl/MACROWRK        S             C
/home/okumura/Mypds/SnSmpl/MACRO           S             C
/home/okumura/Mypds/SnSmpl/FLUX            S             C
/home/okumura/Mypds/SnSmpl/MICREF          S             C
62 45 11  7 /
62(1)      /
45(1)      /
2 2 6 2 3 5 8 8 9 8 9 /
6 6 6 6 6 6 9         /

3 20 20 20 2    2 20  0 0 0   1 0 10 30 0   0 60 0    / Pij Control
0 100 100 5 5 5 -1  0.0001 0.00001 0.001 1.0 10. 0.5  /
19(1) 2    / X-R
19(1) 2    / M-R
0.0  0.950 1.950 17*0.7500 15.0000 / RX
2  / NMAT
FUELX0FX  0  5 3.13150E+02 2.94000E+01 0.0 / FUEL  U= 60.0 G/CC
XH01H001  0  0  6.45244E-02
XN040001  0  0  9.02153E-04
XO060001  0  0  3.49747E-02
XU050001  2  0  1.41980E-04
XU080001  2  0  1.03898E-05
CLDDX0CX  0  7 2.93150E+02 6.00000E-01 0.0 / SUS304
XC020001  0  0  3.17290E-04
XSIN0001  0  0  1.69620E-03
XCRN0001  2  0  1.74080E-02
XMN50001  2  0  1.73430E-03
```

```
XFEN0001  2  0  5.78720E-02
XNIN0001  2  0  8.11160E-03
XS0N0001  0  0  4.45720E-05
0   / PEACO
*************************************************************************
ANIS
WHOLE CORE 107G CALCULATION USING ANISN(S8P1) TO GET CONDENSED X-SEC.
0 0 0 1 0  0 0 0 0 0  0 -2 1 0 2  3 -1 0 0 0 / SRAC CONTROL
1.000E-15 / BUCKLING:NOT EFFECTIVE
15&
1 0 1 8 2  1 0 3 20 1  107 0 0 0 0  0 0 0 0 0  0 0 0 50 0  0 0 0 150 0
0 0 0 0 1  0
16*
0.00000E+00 0.00000E+00 1.00000E-05 1.42089E+00 5.39490E+01
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 5.00000E-01
5.00000E-05 5.00000E-02 1.00000E-02 0.00000E+00
00T
04*
0.0 0.950 1.950 17*0.750 15.000  / MESH BOUNDARY
08&
17(1) 2 2 3    / ZONE BY MESH
09&
   1  1  2    / MATERIAL BY ZONE
19&
   1  1  1    / P1 FOR ALL ZONES
27&
   1  2  3    / X-REGION BY ZONE
00T
2 / NMAT
CELLA012  0  0  0.0  0.0  0.0 / FUEL  U=60.0 G/CC
CELLA022  0  0  0.0  0.0  0.0 / SUS304
*************************************************************************
TWOC
WHOLE CORE 18 G CALCULATION USING TWOTRAN-2 (S8P1)
0 0 0 1 0   0 0 0 0 1   0 3 0 0 2   0 1 0 0 0 / SRAC CONTROL
1.000E-15 / ZERO BUCKLING
1 / NO OF TITLE CARD
WHOLE CORE 18 G CALCULATION USING TWOTRAN-2 (S8P1) : 2D-RZ : FORWARD
0 1 8 18 4   4 1 0 0 0   1 0 3 3 0  0 0 0 0 0    0 0 0 0 0  30 0 0
700 2   0 0 1 2 2  1 3 0 1 0  0 0    / 42I
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 1.00000E-05 1.00000E+00 0.00000E+00 0.00000E+00
 8  5  2  1    / FINE R-MESH
 2 25  2  1    / FINE Z-MESH
0.0   8.00   13.200  14.700  15.000  / R-MESH
0.0   1.50   52.449  53.949  54.249  / Z-MESH
  -2 -2 -2 -3
  -1 -1 -2 -3
  -2 -2 -2 -3
  -3 -3 -3 -3
  16(0)
3 / NMAT
ANISA010  0  0  0.0  0.0  0.0 / INNER FUEL
ANISA020  0  0  0.0  0.0  0.0 / OUTER FUEL
ANISA030  0  0  0.0  0.0  0.0 / SUS304
```

one blank line (null case name to terminate job)

5.4 Three-dimensional diffusion calculation (CITATION)

Figure 5.4-1 shows a three-dimensional X-Y-Z calculation model of a light water reactor for CITATION three-dimensional diffusion module. Not only multiplication factor but also power distribution and one-point kinetics parameters will be calculated. The following is a sample input organized by three cases.

(1) Few group constants for 3.2 wt.% fuel region by PIJ (case name: **`FUL1`**)

A square lattice cell model for a fuel pin of 3.2 wt.% enriched UO_2 is solved by PIJ with 107-group structure to yield two-group constants for the succeeding whole reactor calculation. The diameter of fuel pellet 9.5mm, thickness of cladding 0.65mm and fuel pin pitch 12.6mm are assumed.

The two-group constants for reflector used in the succeeding core calculation are collapsed by using the asymptotic spectrum installed in the library.

(2) Few group constants for 2.1wt.% fuel region by PIJ (case name: **`FUL2`**)

For the fuel pin cell of different enrichment, the same cell calculation is executed. As the geometry is identical with that of the previous case, the input for PIJ is not required by specifying IC11=1.

(3) Core calculation by CITATION (case name: **`CORE`**)

By using the homogenized constants provided by the previous two cases, a whole core calculation of X-Y-Z system is carried out by CITATION. The supposed active core is composed by array of fuel assemblies, each of which has dimension 20cm*20cm*340cm. The outer fuel region is loaded with fuel pins of 3.2 wt.% enriched uranium and the inner with those of 2.1 wt.%. The active core is surrounded by the reflector of the same dimension with fuel assembly. The outer boundary of reflector is assumed as black. In axial direction, the upper and lower reflectors of 20cm thick are installed.

Upon calculation, 1/4 core in horizontal direction and 1/2 in axial direction is solved by using reflective boundary condition owing to the symmetry. A mesh size of 5cm is applied in every direction. By specifying the kinetic parameter calculation option, effective delayed neutron fraction, prompt neutron lifetime and decay constants of precursors will be obtained. Note that the two-group structure in this sample does not yield proper effective delayed neutron fraction. Some calculation scheme such that the fission spectrum of delayed neutron can be reflected on the result may be required.

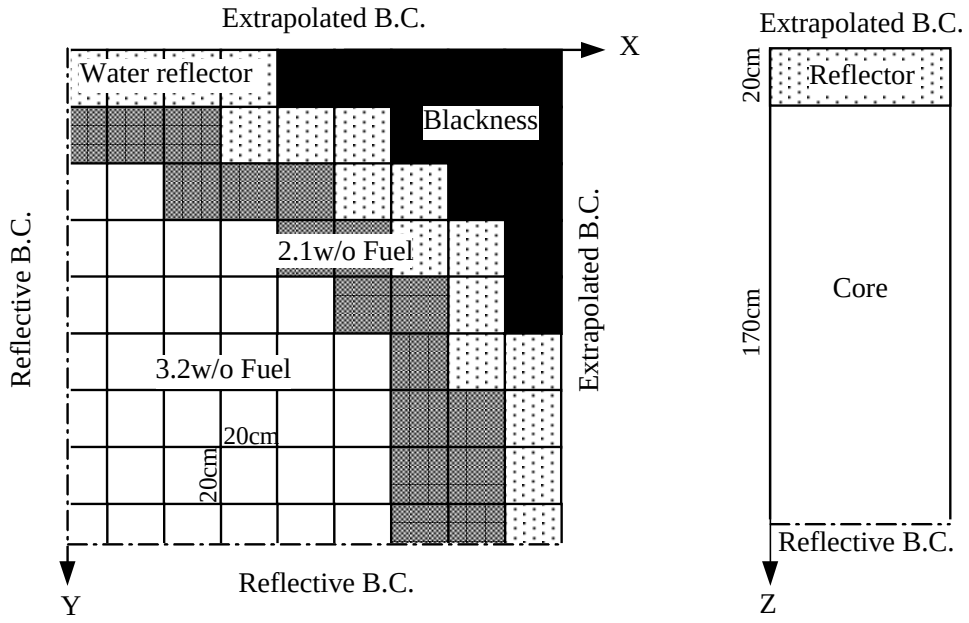


Fig.5.4-1 Core geometry of sample input for 3-D diffusion calculation by CITATION

[File name: CitXYZ.sh]----------

```
FUL1
MACRO FOR INNER FUEL (3.2W/O UO2) BY PIJ
1 1 1 1 2   1 4 3 -2 1   0 0 0 0 2   0 1 0 0 0 / SRAC CONTROL
1.0000E-20 / BUCKLING
/home/okumura/SRACLIB-JDL33/pds/pfast      Old           File
/home/okumura/SRACLIB-JDL33/pds/pthml      O             F
/home/okumura/SRACLIB-JDL33/pds/pmcrs      O             F
/home/okumura/Mypds/CitXYZ/UFAST           Scratch       Core
/home/okumura/Mypds/CitXYZ/UTHERMAL        S             C
/home/okumura/Mypds/CitXYZ/UMCROSS         S             C
/home/okumura/Mypds/CitXYZ/MACROWRK        S             C
/home/okumura/Mypds/CitXYZ/MACRO           S             C
/home/okumura/Mypds/CitXYZ/FLUX            S             C
/home/okumura/Mypds/CitXYZ/MICREF          S             C
61 46   1 1    /
61(1)          /
46(1)          /
61             /
46             /

4 7 7 3 1   1 7 0 0 0   5 0 6 45 0   0 90 0         / PIJ CONTROL
0 100 50 5 5 5 -1  0.0001 0.00001 0.001 1.0 10. 0.5  /
1 1 1 2 3 3 3 /  R-T
3(1)          /  X-R
1 2 3         /  M-R
0.0 0.236714 0.334764 0.41  0.475  0.5267 0.5783 0.630   / RX
4  / NMAT
FUE1X0AX  0 3  900.   0.82     0.0  / 1 : INNER FUEL 3.2W/O
XU050009  2 0  7.2270E-4       /1
XU080009  2 0  2.1585E-2       /2
XO060009  0 0  4.4616E-2       /3
CLD1X0BX  0 3  600.   0.13     0.0  / 2 : CLADDING
XZRN0008  0 0  3.8032E-2       /1
XCRN0008  0 0  6.7152E-5       /2
XFEN0008  0 0  1.3129E-4       /3
MOD1X0CX  0 2  581.   1.0      0.0  / 3 : MODERATOR
```

```
XH01H008  0 0  4.7508E-2      /1
XO060008  0 0  2.3754E-2      /2
REFLX0DX  0 6  581.   1.0     0.0  / 4 : REFLECTOR
XH01H008  0 0  4.7508E-2      /1
XO060008  0 0  2.3754E-2      /2
XFEN0008  0 0  1.7886E-2      /3
XCRN0008  0 0  5.2140E-3      /4
XNIN0008  0 0  2.4294E-3      /5
XMN50008  0 0  2.5977E-4      /6
0  / PEACO
```
FUL2
```
MACRO FOR OUTER FUEL (2.1W/O UO2), SAME GEOMETRY WITH THE ABOVE CASE
1 1 1 1 2   1 4 3 -2 1   1 0 0 0 2   0 1 0 0 0 / SRAC CONTROL
1.0000E-20 / BUCKLING
3  / NMAT
FUE2X0EX  0 3  900.   0.82    0.0  / 1 : OUTER FUEL 2.1W/O
XU050009  2 0  4.7428E-4      /1
XU080009  2 0  2.1831E-2      /2
XO060009  0 0  4.4610E-2      /3
CLD2X0FX  0 3  600.   0.13    0.0  / 2 : CLADDING
XZRN0008  0 0  3.8032E-2      /1
XCRN0008  0 0  6.7152E-5      /2
XFEN0008  0 0  1.3129E-4      /3
MOD2X0GX  0 2  581.   1.0     0.0  / 3 : MODERATOR
XH01H008  0 0  4.7508E-2      /1
XO060008  0 0  2.3754E-2      /2
0  / PEACO
```
CORE
```
SAMPLE FOR CITATION-3D(X-Y-Z), 1/8 CORE
0 0 0 1 0  0 0 0 0 1  0 5 0 0 2  0 1 0 0 0 / SRAC CONTROL
1.0000E-20 / BUCKLING (NOT EFFECTIVE)
3 0 -1 / NM NXR ID
1 1   / IXKY IDELAY (CALCULATE KINETICS PARAMETERS)
5.0CM MESH SIZE IN EACH DIRECTION
EPS(FLUX) < 1.0E-4, EPS(KEFF) < 1.0E-5,  ZONE 4:BLACKNESS
001
  0  0  0  0  0  0  0  0  0  0  0  1  0  0  0  0  0  0  0  0  0  0
  1  0  0  0  0  0  0  0  0  0  0  1  1  0  0  0  0  0  0  0  0  0  0  1
900
  0.
003
  0  0  0  0 11  0  0  0  0  0  1  0  0  1  0  1  4  1  0  0  0  0  0  0
  0.0001    0.00001
  0.0       0.0        3411.0     1.0        0.1250
004
  2 10.00000  4 20.00000  4 20.00000  4 20.00000  4 20.00000  4 20.00000
  4 20.00000  4 20.00000  4 20.00000  0
  4 20.00000  4 20.00000  4 20.00000  4 20.00000  4 20.00000  4 20.00000
  4 20.00000  4 20.00000  2 10.00000  0
  4 20.00000 34 170.0000  0
005
  3  3  3  3  4  4  4  4  4
  3  3  3  3  3  3  4  4  4
  3  3  3  3  3  3  3  4  4
  3  3  3  3  3  3  3  3  4
  3  3  3  3  3  3  3  3  4
  3  3  3  3  3  3  3  3  3
  3  3  3  3  3  3  3  3  3
  3  3  3  3  3  3  3  3  3
  3  3  3  3  3  3  3  3  3    / AXIAL REFLECTOR
  3  3  3  3  4  4  4  4  4
  2  2  2  3  3  3  4  4  4
  1  1  2  2  2  3  3  4  4
  1  1  1  1  2  2  3  3  4
  1  1  1  1  1  2  2  3  4
  1  1  1  1  1  1  2  3  3
  1  1  1  1  1  1  2  2  3
  1  1  1  1  1  1  1  2  3
```

```
  1  1  1  1  1  1  1  2  3    / CORE
008
 -2  1  1
999

1 2 3   / MATTERIAL NO. BY ZONE
3       / NMAT FOR CORE
FUL1A010  0 0    0.0  0.0  0.0   / HOMOGENIZED INNER FUEL
FUL2A010  0 0    0.0  0.0  0.0   / HOMOGENIZED OUTER FUEL
REFLA0D0  0 0    0.0  0.0  0.0   / REFLECTOR
```

one blank line (null case name to terminate job)

5.5 BWR Fuel Assembly Calculation (PIJ)

As the last sample, an example to analyze a fuel assembly of BWR loaded with MOX by using a geometry model (IGT=16) of PIJ. The assembly is shown in Fig.5.5-1 at the last of this section. A series of calculations consists of the following 6 cases.

(1) A MOX fuel pin cell calculation (case name: **UPIN**)

A pin cell calculation by PIJ (IGT=4) with 107-group structure is solved for the MOX pin cell with the model shown in Fig.5.5-2. The cross-sections are homogenized in the cell and collapsed into 39-group structure.

(2) A partial cell containing a UO_2-Gd_2O_3 pin (case name: **GDPN**)

A 3×3 rod cell calculation by PIJ (IGT=9) with 107-group structure is done by using the model shown in Fig.5.5-3 to obtain the 39-group constants of UO_2-Gd_2O_3 rod under the condition that it is surrounded by MOX pins. As the later assembly calculation treat UO_2-Gd_2O_3 rod heterogeneously, the cross-sections of meat, cladding and moderator are separately collapsed by assigning different X-Region number.

(3) A partial cell of control rod insertion (case name: **CRIN**)

Control blade is heterogeneously treated with the cell model shown in Fig.5.5-4. The homogenized cross-sections of the control blade are obtained in 39-group structure by PIJ (IGT=16).

(4) A partial cell of control rod withdrawn (case name: **CROT**)

The same geometry as the previous case is treated while the materials inside control blade are replaced by saturated water used in gap region.

(5) An assembly calculation with control rod insertion (case name: **ASMI**)

By using the 39-group constants obtained in (1), (2) and (3) cases, an eigenvalue problem is solved by PIJ with 39-group structure for the assembly with control rod insertion. Fig.5.5-5 shows the R-Region map (identical with T-Region map) used in the calculation where the thick water rod is treated as homogeneous mixture because of the restriction of the model IGT=16.

(6) An assembly calculation with control rod withdrawal (case name: **ASMO**)

The same problem as the previous case is solved with the replacement of cross-sections for the control blade obtained in (3) by those in (4).

Note: This sample is time consuming and it is necessary to make a load module of enlarged array size by changing defaulted parameters in the include files.

- Shell-script to make users own load module: ~SRAC/tool/lmmake/lmmk/lmml.sh
- Include files: ~SRAC/tool/lmmake/lmmk/lmml.sh
- Suggested parameter values described in include file: ~SRAC/tool/lmmake/lmmk/lmml.sh

```
MAINSINC:  PARAMETER (MXSIZE=7000000)
PIJPMINC:  PARAMETER (MEMPIJ= 2 0000,MXMESH=300,MXNTAB=3000)
```

[File name: BWR.sh]----------

```
UPIN
Unit MOX Fuel Pin
1 1 1 1 2   1 4 3 -2 1   0 0 0 0 2   0 -1 0 0 0 / SRAC Control
1.000E-20 / Geometrical buckling for P1/B1 calculation
/home/okumura/SRACLIB-JDL33/pds/pfast      Old           File
/home/okumura/SRACLIB-JDL33/pds/pthml      O             F
/home/okumura/SRACLIB-JDL33/pds/pmcrs      O             F
/home/okumura/Mypds/BWR/UFAST              Scratch       Core
/home/okumura/Mypds/BWR/UTHERMAL           S             C
/home/okumura/Mypds/BWR/UMCROSS            S             C
/home/okumura/Mypds/BWR/MACROWRK           S             C
/home/okumura/Mypds/BWR/MACRO              S             C
/home/okumura/Mypds/BWR/FLUX               S             C
/home/okumura/Mypds/BWR/MICREF             S             C
62 45 20 19            /  107g => 20+19=39g
62(1)                 /
45(1)                 /
10 10 10 7 8  2 2 13(1)  /
3 15(2) 4 4 4           /
***** Enter one blank line after input for energy group structure

***** Input for PIJ (Collision Probability Method)
4 7 7 3 1  1 7 0 0 0  5 0 6 23 0  0 45 0   / Pij Control
0 100 50 5 5 5 -1  0.0001  0.00001  0.001  1.0 10. 0.5
1 1 1  2  3 3 3       / R-T
1 1 1                 / X-R
1 2 3                 / M-R
0.0 0.3054 0.4319 0.529  0.615  0.682 0.748 0.815  / RX
****** Input for material specification
3 / NMAT
MOX1X01X  0  8  900.0   1.058  0.0  / MOX Pellet
XU050009  2  0  4.40524E-05
XU080009  2  0  2.17045E-02
XPU90009  2  0  6.73856E-04
XPU00009  2  0  3.18053E-04
XPU10009  2  0  1.30771E-04
XPU20009  2  0  7.76602E-05
XAM10009  2  0  5.99868E-06
XO060009  0  0  4.59098E-02
ZR21X02X  0  1  600.0   0.172  0.0  / Cladding for MOXl Pin
XZRN0008  0  0  4.32418E-02
H2O1X03X  0  2  600.0   0.0    0.0  / Moderator(42%Void)
XH01H008  0  0  2.96967E-02
XO060008  0  0  1.48483E-02
0 / PEACO
************************************************************************
GDPN
3*3 Array with UO2-Gd2O3 Rod in Center (IGT=9)
1 1 1 1 2   1 4 3 -2 1   0 0 0 0 2   0 -1 0 0 0 / SRAC Control
```

```
1.000E-20 / Geometrical buckling for P1/B1 calculation
***** Input for PIJ (Collision Probability Method)
9 36 14 6 4   0 3 0 0 3   2 0 6 23 5   0 45 0  / Pij Control
0 100 50 5 5 5 -1  0.0001  0.00001  0.001  1.0 10. 0.5
10 14 10 6 14  10 7 7 7 8  9 11 11 11 12  13 7 7 7 8
9 1 2 3 4  5 11 11 11 12  13 7 7 7 8  9  / T-S
1 1 1 2 3  3 4 5 6 6  4 5 6 6  /  R-T
1 2 3 4 4  4                  /  X-R
1 2 3 4 5  6                  /  M-R
0.0 3*1.63         /  RX
0.815 2*1.63       /  RPP
6(0.0 0.3054 0.4319 0.529  0.615  0.715)  / RDP
&15 2 1  / Plot Geometry
6 / NMAT
GDUOX04X  0  9  900.0   1.058  0.0  / 1: UO2-Gd2O3(4.5wt%)
XU050009  2  0  7.66040E-04
XU080009  2  0  2.11208E-02
XO060009  0  0  4.60776E-02
XGD40009  2  0  3.23186E-05
XGD50009  2  0  2.27770E-04
XGD60009  2  0  3.17031E-04
XGD70009  2  0  2.41621E-04
XGD80009  2  0  3.81668E-04
XGD00009  2  0  3.35498E-04
ZR22X05X  0  1  600.0   0.172  0.0  / 2: Cladding for Gd2O3-UO2
XZRN0008  0  0  4.32418E-02
H2O2X06X  0  2  600.0   0.0    0.0  / 3: Moderator around Gd2O3-UO2
XH01H008  0  0  2.96967E-02
XO060008  0  0  1.48483E-02
MOX2X07X  0  8  900.0   1.058  0.0  / 4: MOX Fuel
XU050009  2  0  4.40524E-05
XU080009  2  0  2.17045E-02
XPU90009  2  0  6.73856E-04
XPU00009  2  0  3.18053E-04
XPU10009  2  0  1.30771E-04
XPU20009  2  0  7.76602E-05
XAM10009  2  0  5.99868E-06
XO060009  0  0  4.59098E-02
ZR23X08X  0  1  600.0   0.172  0.0  / 5: Cladding for UO2 fuel Pin
XZRN0008  0  0  4.32418E-02
H2O3X09X  0  2  600.0   0.0    0.0  / 6: Moderator around UO2 Pin
XH01H008  0  0  2.96967E-02
XO060008  0  0  1.48483E-02
0 / PEACO
*************************************************************************
CRIN
Control-Blade with B4C Powder (Rod In)
1 1 1 1 0   1 4 0 -2 1   0 0 0 0 2   0 -1 0 0 0 / SRAC Control
1.000E-20 / Geometrical buckling for P1/B1 calculation
***** Input for PIJ (Collision Probability Method)
16 15 12 9 6   1 1 13 1 0   3 0 10 43 2   1 90 0  / Pij Control
0 100 50 5 5 5 -1  0.0001  0.00001  0.001  1.0 10. 0.5
3 4 5 6 7   8 9 10 10 11   11 12 12 1 2  / T-S
1 2 3 4 5   6 7 8 8 9   9 9    / R-T
1 1 1 1 2   3 4 5 6            / X-R
1 2 3 4 3   5 6 7 8            / M-R
0.0 0.29   / RX
0.0 0.29 0.4 1.05 1.1525 1.48 8*0.815 / TY
2  / IXP
1  / IYP
0.0 0.21 0.28 / RDP
****** Input for material specification
8 / NMAT
B4CPX0AX  0  3  600.0 0.0  0.0 / 1:B4C Pellet(Nat.B and 70%T.D)
XB000008  0  0  1.50776E-02
XB010008  0  0  6.12203E-02
XC020008  0  0  1.90745E-02
CLABX0BX  0  4  600.0 0.0  0.0 / 2:Cladding for Absorber
```

```
XCRN0008  0  0  1.55546E-02
XNIN0008  0  0  9.72490E-03
XMON0008  0  0  1.24036E-03
XFEN0008  0  0  5.83534E-02
SATWX0CX  0  2  600.0 0.0  0.0 / 3:Moderator(Sat.Water)
XH01H008  0  0  4.94151E-02
XO060008  0  0  2.47075E-02
SHEAX0DX  0  4  600.0 0.0  0.0 / 4:Outer Sheath for Control Blade
XCRN0008  0  0  1.55546E-02
XNIN0008  0  0  9.72490E-03
XMON0008  0  0  1.24036E-03
XFEN0008  0  0  5.83534E-02
CHBXX0EX  0  4  600.0 0.0  0.0 / 5:Channel Box
XZRN0008  0  0  4.24851E-02
XFEN0008  0  0  1.05945E-04
XSNN0008  0  0  5.14929E-04
XCRN0008  0  0  7.58618E-05
H2O4X0FX  0  2  600.0 0.0  0.0 / 6:Moderator(42%Void) for Clearance
XH01H008  0  0  2.96967E-02
XO060008  0  0  1.48483E-02
UPINX01X  0  0  0.0  0.0  0.0  / 7:Homogenized Fuel near Channel Box
UPINX01X  0  0  0.0  0.0  0.0  / 8:Homogenized Fuel
*************************************************************************
CROT
Control-Blade with B4C Powder (Rod out)
1 1 1 1 0   1 4 0 -2 1   1 0 0 0 2   0 -1 0 0 0 / SRAC Control
1.000E-20 / Geometrical buckling for P1/B1 calculation
****** Input for material specification
8 / NMAT
SATWX0CX  0  0  0.0  0.0  0.0  / 1:Moderator(Sat.Water):B4C Replaced
SATWX0CX  0  0  0.0  0.0  0.0  / 2:Moderator(Sat.Water):Clad Replaced
SATWX0CX  0  0  0.0  0.0  0.0  / 3:Moderator(Sat.Water)
SATWX0CX  0  0  0.0  0.0  0.0  / 4:Moderator(Sat.Water):Sheath Replaced
CHBXX0EX  0  0  0.0  0.0  0.0  / 5:Channel Box
H2O4X0FX  0  0  0.0  0.0  0.0  / 6:Moderator(42%Void) for Clearance
UPINX01X  0  0  0.0  0.0  0.0  / 7:Homogenized Fuel near Channel Box
UPINX01X  0  0  0.0  0.0  0.0  / 8:Homogenized Fuel
*************************************************************************
ASMI
8*8 ABWR Fuel Assembly with Control Blade by PIJ
1 0 0 1 0   1 0 0 0 1   0 1 0 0 2   0 1 0 0 0  / SRAC Control
1.000E-20 / Geometrical buckling for P1/B1 calculation
***** Input for PIJ (Collision Probability Method)
16 649 219 219 1  1 25 25 12 0  2 0 6 23 2  1 45 0   / Pij Control
0 100 50 5 5 5 -1  0.0001  0.0001  0.001  1.0 10. 0.5
  28  29  30  30  31   1   1   2   2   3   3   4   4   5   5   6   6   7
   8  32  32  34  35  35  36
  29  37  38  38  39  40  41  42  42  43  43  44  44  45  45  46  46  47
  47  48  49  50  51  51  52
  30  38   9   9  10  10  10  11  11  12  12  13  13  14  14  15  15  16
  16  16  17  17  18  18  53
  30  38   9  64  65  65  65  66  66  67  67  68  68  69  69  70  70  71
  71  72  73  74  75  18  53
  31  39  10  65  86  86  87  89  89  92  92  94  94  97  97 100 100 102
 102 102 105 106  76  19  54
   1  40  10  65  86  86  87  89  89  92  92  94  94  97  97 100 100 102
 102 102 105 106  76  19  54
   1  41  10  65  87  87  88  90  91  93  93  95  96  98  99 101 101 103
 104 104 107 108  77  19  54
   2  42  11  66  89  89  90 109 110 174 175 112 113 116 117 178 179 120
 121 121 124 125  78  20  55
   2  42  11  66  89  89  91 110 111 176 177 114 115 118 119 180 181 122
 123 123 126 125  78  20  55
   3  43  12  67  92  92  93 174 176 127 128 130 131 182 183 134 135 186
 187 187 138 139  79  21  56
   3  43  12  67  92  92  93 175 177 128 129 132 133 184 185 136 137 188
 189 189 140 139  79  21  56
   4  44  13  68  94  94  95 112 114 130 132 198 199 201 202 190 191 141
```

```
 142 142 145 146  80  22  57
   4  44  13  68  94  94  96 113 115 131 133 199 200 203 204 192 193 143
 144 144 147 146  80  22  57
   5  45  14  69  97  97  98 116 118 182 184 201 203 205 206 148 149 194
 195 195 152 153  81  23  58
   5  45  14  69  97  97  99 117 119 183 185 202 204 206 207 150 151 196
 197 197 154 153  81  23  58
   6  46  15  70 100 100 101 178 180 134 136 190 192 148 150 155 156 158
 159 159 162 163  82  24  59
   6  46  15  70 100 100 101 179 181 135 137 191 193 149 151 156 157 160
 161 161 164 163  82  24  59
   7  47  16  71 102 102 103 120 122 186 188 141 143 194 196 158 160 165
 166 166 168 169  83  25  60
   8  47  16  71 102 102 104 121 123 187 189 142 144 195 197 159 161 166
 167 167 170 169  83  25  60
  32  48  16  72 102 102 104 121 123 187 189 142 144 195 197 159 161 166
 167 167 170 169  83  25  60
  33  49  17  73 105 105 107 124 126 138 140 145 147 152 154 162 164 168
 170 170 171 172  84  26  61
  34  50  17  74 106 106 108 125 125 139 139 146 146 153 153 163 163 169
 169 169 172 173  84  26  61
  35  51  18  75  76  76  77  78  78  79  79  80  80  81  81  82  82  83
  83  83  84  84  85  27  62
  35  51  18  18  19  19  19  20  20  21  21  22  22  23  23  24  24  25
  25  25  26  26  27  27  62
  36  52  53  53  54  54  54  55  55  56  56  57  57  58  58  59  59  60
  60  60  61  61  62  62  63
& 25x25 Grid
        208 214              209 215
 208 214              210 216        211 217
                           212 218
        210 216                     213 219
 209 215        212 218
        211 217        213 219
& 12 Gd PIN /  T-S
219(1)      /  X-R
 8(5)     & Control Blade (Satulated Water when Control rod out)
19(7)     & Channel Box
 4(10)    & Central Structure of Control Blade
32(6)     & Flow Area out of Channel(Satulated Water)
22(8)     & Void Water inside Channel (next to Channel Box)
23(1)     &  Homogenized Fuel (MOX)
15(1)   3(1)  &  MOX and Outer MOX
11(1)   3(1)
 4(1)   3(1)
 4(1)   3(1)
 7(1)   3(1)
 3(1)   3(1)
        3(1)
24(4)     & Void Water inside Channel (next to Gd Pin)
10(9)     & Water Rod
 6(2)     & Gd2O3-UO2 Fuel
 6(3)     & Cladding of Gd Pin   (End of M-R)
0.0   1*0.4   1*0.65  1*0.1025  1*0.3275
      2.26 2.295 1*0.815     & 1st column fuel
      10*0.815               & 2nd - 6th column fuel
      1*0.815 12.7 12.89     & 7th column fuel
      2*0.815                & 8th column fuel
      1*0.3275  1*0.1025  1*0.55   / RX
0.0   1*0.4   1*0.65  1*0.1025  1*0.3275
      2.26 2.295 1*0.815     & 1st row fuel
      10*0.815               & 2nd - 6th row fuel
      1*0.815 12.7 12.89     & 7th row fuel
      2*0.815                & 8th row fuel
      1*0.3275  1*0.1025  1*0.55     / TY
11 17  9 15 19 17 11 19  9 13 11 15 / IXP
 9  9 11 11 11 13 15 15 17 17 19 19 / IYP
12(0.0 0.529 0.615) / RDP
```

```
****** Input for material specification
10 / NMAT
UPINX01X  0  0  0.0  0.0  0.0  / 1:Fuel Region of MOX Pin
GDPNX01X  0  0  0.0  0.0  0.0  / 2:Fuel Region of Gd2O3-UO2 Pin
GDPNX02X  0  0  0.0  0.0  0.0  / 3:Cladding for Gd2O3-UO2 Pin
GDPNX03X  0  0  0.0  0.0  0.0  / 4:Moderator(42%Void) near Gd Pin
CRINX01X  0  0  0.0  0.0  0.0  / 5:Control Rod Blade
CRINX02X  0  0  0.0  0.0  0.0  / 6:Wide Gap (Sat.Water)
CRINX03X  0  0  0.0  0.0  0.0  / 7:Channel Box
CRINX04X  0  0  0.0  0.0  0.0  / 8:Clearance Void Water
WTRDX0GX  0  3  600.0 0.0  0.0 / 9:Water Rod
XZRN0008  0  0  3.64312E-03    /  Clad(8.425%)+(Water(42%void)(91.575%))
XH01H008  0  0  2.71948E-02
XO060008  0  0  1.35973E-02
CSTRX0HX  0  4  600.0 0.0  0.0 / 10:Central Structure of Control Blade
XCRN0008  0  0  1.55546E-02
XNIN0008  0  0  9.72490E-03
XMON0008  0  0  1.24036E-03
XFEN0008  0  0  5.83534E-02
**************************************************************************
ASMO
8*8 ABWR Fuel Assembly without Control Blade by PIJ
1 0 0 1 0   1 0 0 0 1   1 1 0 0 2   0 1 0 0 0  / SRAC Control
1.000E-20 / Geometrical buckling for P1/B1 calculation
****** Input for material specification
10 / NMAT
UPINX01X  0  0  0.0  0.0  0.0  / 1:Fuel Region of MOX Pin
GDPNX01X  0  0  0.0  0.0  0.0  / 2:Fuel Region of Gd2O3-UO2 Pin
GDPNX02X  0  0  0.0  0.0  0.0  / 3:Cladding for Gd2O3-UO2 Pin
GDPNX03X  0  0  0.0  0.0  0.0  / 4:Moderator(42%Void) near Gd Pin
CROTX01X  0  0  0.0  0.0  0.0  / 5:Control Rod Blade Replaced by Sat.Water
CROTX02X  0  0  0.0  0.0  0.0  / 6:Wide Gap (Sat.Water)
CROTX03X  0  0  0.0  0.0  0.0  / 7:Channel Box
CROTX04X  0  0  0.0  0.0  0.0  / 8:Clearance Void Water
WTRDX0GX  0  0  0.0  0.0  0.0  / 9:Water Rod
CROTX02X  0  0  0.0  0.0  0.0  / 10:Central Structure Replaced by Sat.Water
```

one blank line (null case name to terminate job)

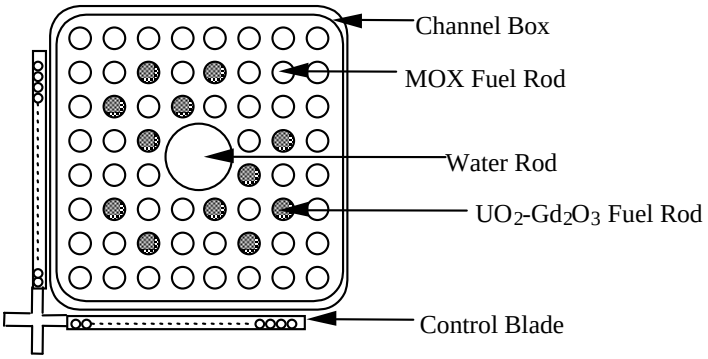


Fig.5.5-1 Geometry of sample input for BWR fuel assembly calculation by PIJ: (BWR.sh)

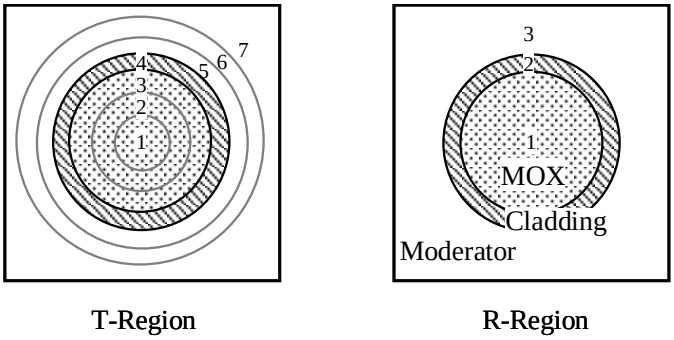


Fig.5.5-2 Unit pin cell calculation model by PIJ (IGT=4) to obtain homogenized cross-sections of MOX fuel cell (case:UPIN)

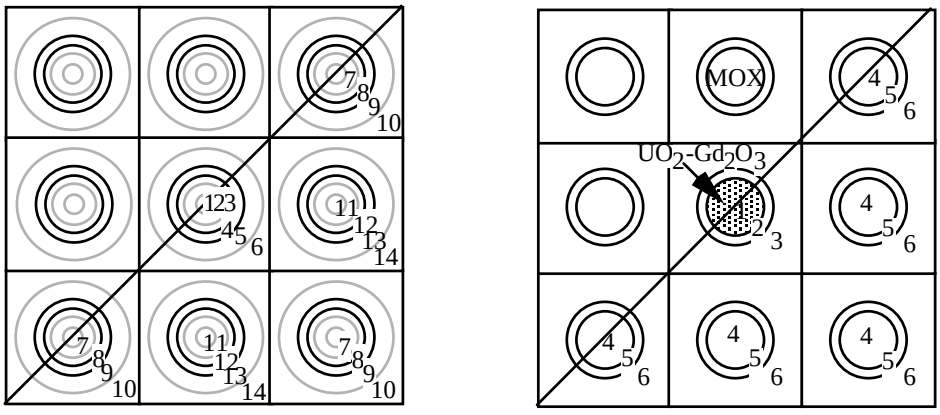


Fig.5.5-3 Multi-cell model by PIJ (IGT=9) to obtain homogenized cross-sections of poisoned fuel cell (case:GDPN)

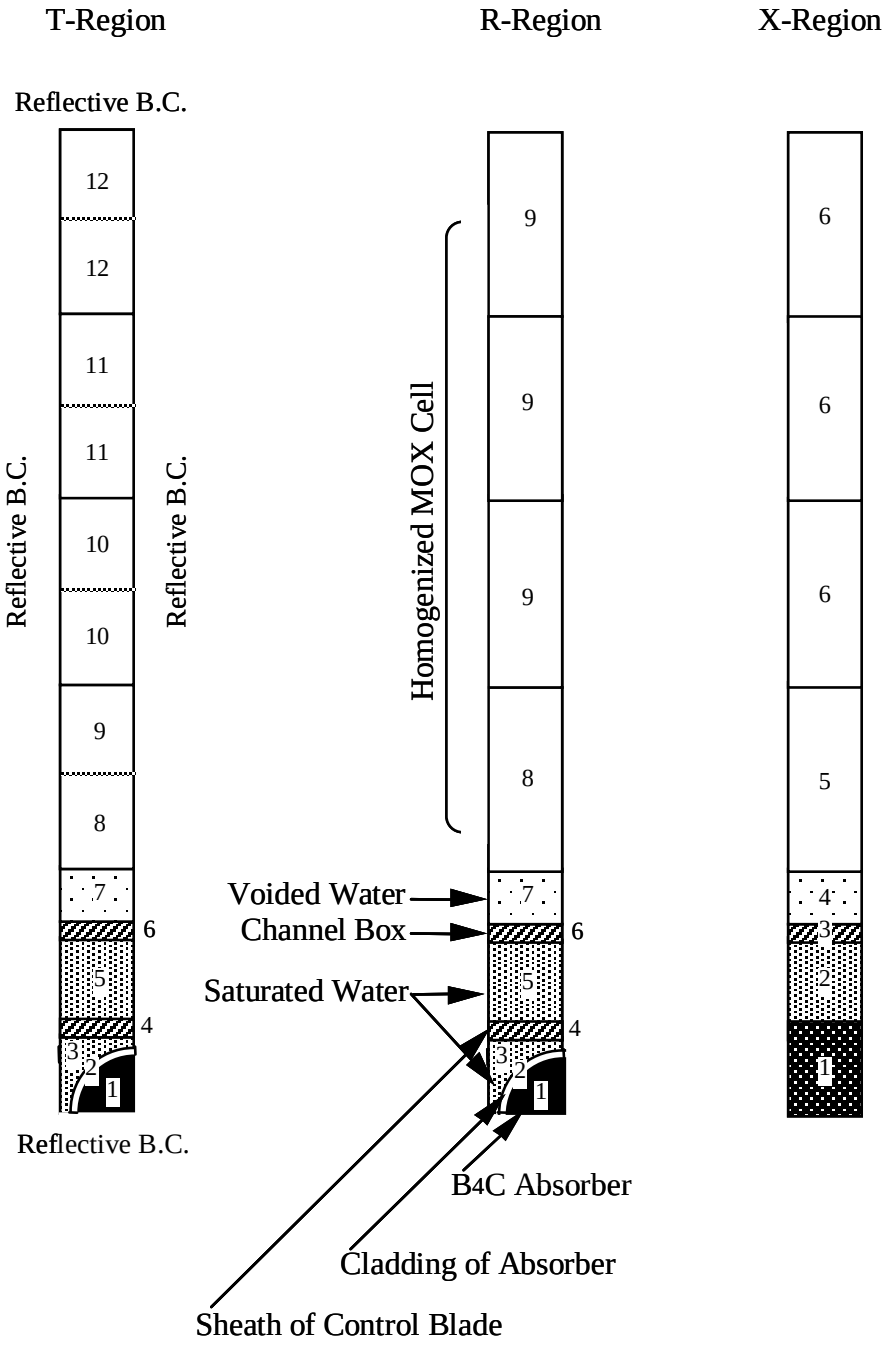
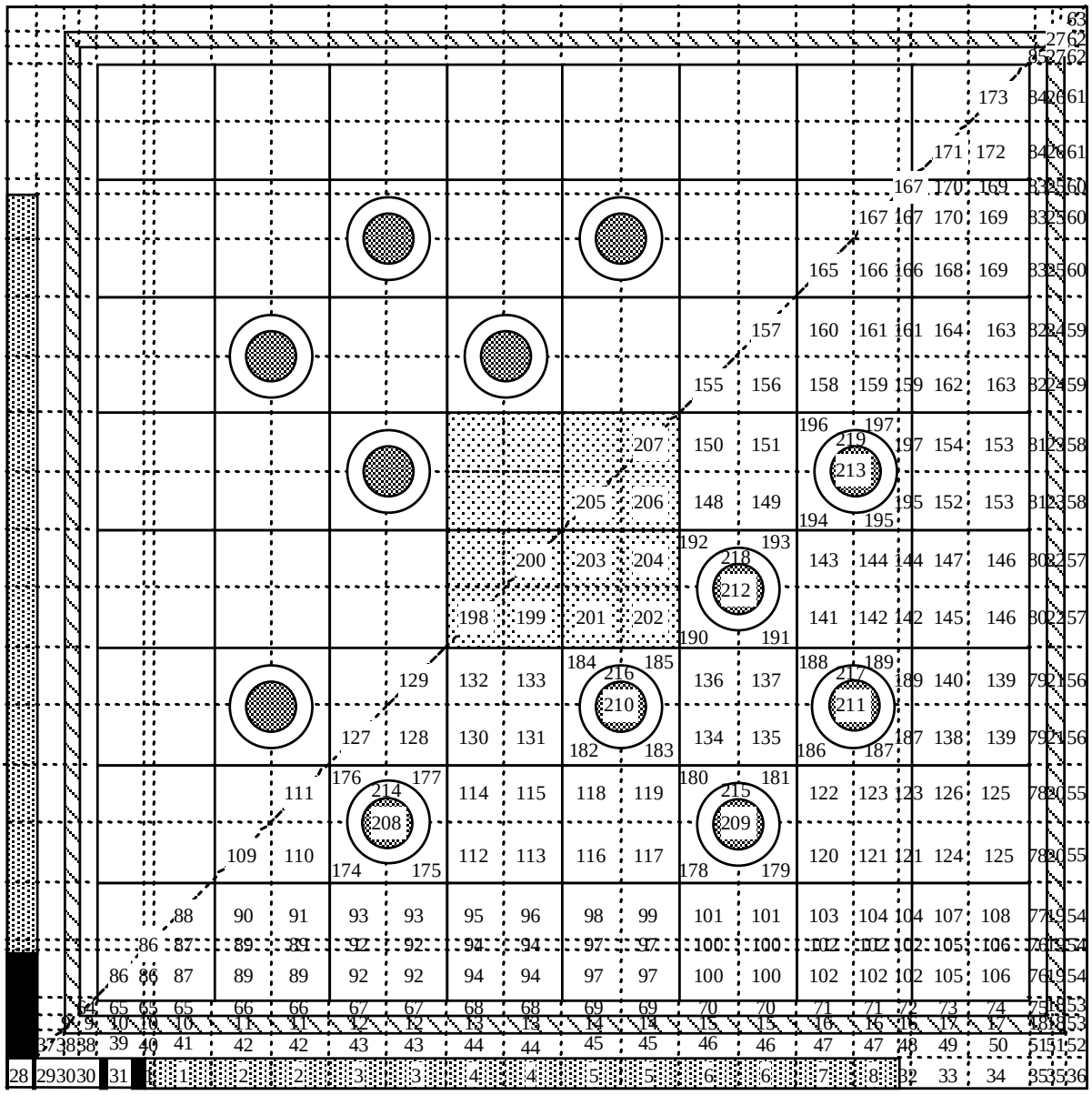


Fig.5.5-4 Multi-cell model by PIJ (IGT=16) to obtain homogenized control blade cell (case:CRIN)



1~8 : Homogenized control rod blade
9~27 : Channel box
28~31 : Central structure of control rod
32~63 : Saturated water (water gap)
64~85 : Voided water near channel box
86~173 : Homogenized MOX cell
174~197 : Voided water around Gd-rod
198~207 : Homogenized water rod
208~213 : UO_2-Gd_2O_3 fuel
214~219 : Cladding of Gd-Rod

Fig.5.5-5 Multi-cell model by PIJ (IGT=16) for a BWR fuel assembly calculation (case:ASMI)

6. Utility for PDS File Management

Printed information on the 99th device may be insufficient for the user's demand or may be not convenient for tabulation and plotting. In the PDS files such as FLUX, MACRO, MACROWRK, and MICREF, a lot of information is stored as binary data. Here, several utilities to extracting necessary information from PDS files are shown.

6.1 PDSTOTXT and TXTTOPDS

(1) PDSTOTXT [~SRAC/util/pdscnvt/shr/pdstotxt.sh]

The PDSTOTXT is a program to convert the content of a member in PDS file into a text file. It is used to dump the contents of members in PDS file or to transfer the members into a machine of different data organization.

(2) TXTTOPDS [~SRAC/util/pdscnvt/shr/txttopds.sh]

The TXTTOPDS is a utility program to reconvert a text file converted by PDSTOTXT into PDS file.

By using PDSTOTXT and TXTTOPDS, it is available to transfer PDS files between machines with different data organization. By these utilities, Public libraries and MACRO files of SRAC can be easily transferred from a machine to others.

6.2 PDSMDL

The PDSMDL (PDS modular subroutine package) is not a complete program but a group of modular subroutines for the user to edit the contents of a member of PDS file. The user makes a main program where the suitable subroutine(s) is (are) called by CALL statement so that the user can read in an array from a member into his defined array, or update the contents of a member. The user who is acquainted with FORTRAN and PDS file in SRAC can utilize these modules in a wide range of applications such as calculation of the reaction rate of arbitrary reaction and transfer of cross-sections into another code, etc. The current library includes 13 modules. The usage including the meaning of arguments are described in the source program of each module [~SRAC/util/pdsmdl/modl/*.f].

(1) ENGEDT

To read in the information on energy group structure from the member CONTe00p stored in MACRO, FLUX, or MICREF file and to transfer to MAIN routine.

(2) ENGWRT

To write the information on energy group structure given by MAIN routine into a PDS file.

(3) FLXEDT

To read in the flux in FLUX file and to transfer to MAIN routine.

(4) FLXWRT

To write the information on neutron flux given by MAIN routine into a PDS file in the format of FLUX file.

(5) MACEDT

To read in the macroscopic cross-sections from the member stored in MACRO or MACROWRK file and to transfer to MAIN routine.

(6) MACWRT

To write macroscopic cross-sections given by MAIN routine into a PDS file in the format of MACRO (MACROWRK) file.

(7) BNPEDT

To read material-wise burn-up information from the member caseBNUP stored in MACRO or MACROWRK file and to transfer to MAIN routine.

(8) BNPWRT

To write material-wise burn-up information given by MAIN routine into a PDS file in the format of MACRO (MACROWRK).

(9) DNTEDT

To read X-Region-wise burn-up information from the member caseDNxT stored in MACRO or MACROWRK file and to transfer to MAIN routine

(10) DNTWRT

To write X-Region-wise burn-up information given by MAIN routine into a PDS file in the format of MACRO (MACROWRK).

(11) MICEDT

To read in the microscopic cross-sections from the member stored in MICREF file and to transfer to MAIN routine.

(12) DLYEDT

To read in the information on delayed neutron of the specified nuclide from the member `Yzzm0000` stored in FASTP library and to transfer to MAIN routine.

(13) FASTLB

To read in the information on energy group structure of Public library from the member `FASTLIB` stored in FASTP library to transfer to MAIN routine.

There exist several routines other than the above which are commonly used for PDS file access such as PDSIN, PDSLN, PDSNM, PDSRD, PDSRM, PDSSR, and PDSWT. However, the user does not need to be aware of function of each routine.

As each of the modules has print monitor option, the user can edit the content of the accessed member in a tabulated form. This option can be utilized for confirmation of the content and debugging of the main routine provided by the user himself.

The modules named by EDT in the tail use read only file, then the file is never damaged. Contrary, the modules named WRT in the tail create new members, and cross-sections given by the main routine are stored in a PDS file for the later use by SRAC.

There are several sample MAIN programs in the directory [~SRAC/util/pdsmdl/main/*/]. After the main routine is made, the load module can be created by compile-linkage together with the module(s) and PDS access routines. Sample Makefile files to make his load module are also there in the same directory. The execution of the load module created with the sample is shown in the next section.

6.3 Other utility programs

The following utility programs are available. Since all of the programs utilize PDSMDL, user can easily modify the programs if necessary.

(1) MACROEDIT [~SRAC/SRAC/util/pdsmdl/shr/MacroEdit.sh]

The MACROEDIT is a utility program to print out the content of the member of macroscopic cross-section file MACRO or MACROWRK. While the direct use of PDSTOTXT for this purpose gives simply printout of one-dimensional array, the use of this MACROEDIT gives tabulated form of macroscopic cross-sections.

(2) MICROEDIT [~SRAC/SRAC/util/pdsmdl/shr/MicroEdit.sh]

The MICROEDIT is a utility program to print out the content of the member of microscopic cross-section file MICREF. It is used for the same purpose as MACROEDIT but for microscopic cross-sections.

(3) FLUXEDIT [~SRAC/SRAC/util/pdsmdl/shr/FluxEdit.sh]

The FLUXEDIT is a utility program to print out the content of the member storing neutron flux of fine or coarse group structure. The flux in FLUX is multiplied by the region volume. The volume can be also printed out in addition to the neutron spectrum and its spatial distribution in a tabular form. The usage is almost the same as to use MACROEDT.

(4) BNUPEDT [~SRAC/SRAC/util/pdsmdl/shr/BnupEdit.sh]

The BNUPEDT is a utility program to print out the information on burn-up calculation (members `caseBNUP` and `caseDNxT`) on MACRO or MACROWRK file. The major results of burn-up calculation written on logical unit 98 are reproduced by BNUPEDIT.

(5) FLUXPLOT [~SRAC/SRAC/util/pdsmdl/shr/ FluxPlot.sh]

The FLUXPLOT is a utility program to provide a table in text form for plotting the neutron spectrum in histogram (log-log) style graph by reading the energy group structure and flux on FLUX file. Actual plotting is done with a spreadsheet software on the market by feeding the table provided by FLUXPLOT.

7. Mathematical Formulations

7.1 Formulations of Collision Probabilities

We present in this section the formulations to evaluate the collision probabilities for a multi-region cell expressed by either of three one-dimensional coordinate systems (plane, sphere and cylinder) or two-dimensional cylindrical coordinates. They are expressed in a form suitable to apply a numerical scheme “Ray-Trace” method developed by Tsuchihashi[33].

Description of this chapter will be started by the derivation of the linear equation to solve the Boltzmann equation by the collision probability method (CPM) then followed by the formulations of collision probabilities in various coordinate systems, in which care is paid to evaluate the surface problem and also the directional probabilities to yield the anisotropic diffusion coefficients.

For the slab geometry, the formulation of the ordinary collision probabilities expressed by the E_{i3} function has been given by Honeck[34] starting from the plane transport kernel by E_{i1} function. Here, we shall start from the basic point kernel, operate first, the double integration along a neutron path (line), finally, achieve the angular integration to yield the general form of the directional collision probabilities expressed by the integral exponential function E_{in}.

For the one-dimensional cylinder, the formulation derived by Takahashi[35] needs that the angular integration to scan the collision regions be repeated for each source region. The similar formulation by Honeck used in the THERMOS code[34] approximates the attenuation of neutron emitted from a source region by that from the mid-point of the source region. This approximation could be covered by sub-dividing the system into so many concentric regions. The formulation given in this chapter is a special case of the general two-dimensional cylinder. For an annular geometry, no integration over the azimuthal angle is needed. The main difference between the present formulation and the formers’ is in the sequence and the coordinates for the integration. Owing to the variable transformation, the angular integration appearing in the formers’ is replaced by the integration over the volume element $d\rho$ where ρ is the distance from the center to one of the parallel lines drawn across the system. The number of lines drawn for the integration is quite small compared with that of the THERMOS code to have the same measure of accuracy, partly because no repeated integration by source region is required, partly because the analytic integration along the line in the source region does not need so many sub-division of the system.

The formulation for collision probabilities in the spherical system which can be sub-divided into an arbitrary number of spherical shells has been given by Tsuchihashi & Gotoh[36] in the course of

studying the resonance absorption of coated particles in the HTGR, while the escape probability for an isolated sphere by Case *et al.*[27] and for a special case of the pebble bed type HTGR by Teuchert[37] have been derived. It will be seen that the final form of the present formulation is quite similar to that of the cylindrical case.

Two-dimensional geometry has been studied, first, by Fukai[38] in his exact expression for collision probabilities in a regular lattice of unit pin rod cell. His expression has been applied to the cluster system with regular array of pin rods by Amyot & Benoist in the PROCOPE code[39]. Fukai's expression is characterized by the numerical process to organize the ranges of double integration for each pair of pin rods between which the interaction is computed. This method requires so much sophisticated programming technique that any sub-division of coolant region has not yet been realized.

An alternate formulation has been presented by Takahashi & Nakayama[40] for the collision probabilities in square and hexagonal lattice cells which was incorporated in a thermalization code GRAFA[41], and also independently by Carlvik[42] for an annularly arrayed pin rod cluster within a cylindrical channel which was realized in a code CLUCOP and a British code PIJ.[43] In their integral formulation to compute the collision probabilities, sets of parallel lines are drawn across the system, and all intersections with region boundaries are determined and the segments of the lines in each region are measured.

Their formulation has been generalized in the treatment of outer boundary conditions, and a numerical scheme for the multi-group calculation, named "Ray-Trace" method has been established by Tsuchihashi during his works to develop the PATH-C code[44] for square and hexagonal array of pin rod cells with a two-dimensional sub-division. This method has been successively applied to the CLUP code[45] for an annularly arrayed pin rod cluster such as used in the ATR, the CLUP77 code[46] for the cluster of BWR geometry, and the CLUPH code[47] for the fuel block of the HTTR.

7.1.1 General Theory

We start at the general expression to describe the behavior of neutrons in a steady state. The neutron angular flux $\varphi(\boldsymbol{r}, \overline{\Omega}, E)$ at position $\boldsymbol{r}$, along direction $\overline{\Omega}$ with energy E satisfies the integral form of the Boltzmann transport equation,

$$\begin{aligned} \varphi(\boldsymbol{r}, \overline{\Omega}, E) = & \int_0^\infty dR \exp(-\overline{\Sigma R}) \\ & \times \left[\int_0^\infty dE' \int_{4\pi} d\overline{\Omega}' \Sigma_s(\boldsymbol{r}', \overline{\Omega}' \to \overline{\Omega}, E' \to E) \varphi(\boldsymbol{r}', \overline{\Omega}', E') + S(\boldsymbol{r}', \overline{\Omega}, E) \right] , \end{aligned} \tag{7.1-1}$$

where R is the distance between point $\boldsymbol{r}$ and $\boldsymbol{r}'$, $\overline{\Omega}$ is the directional vector given by $\overline{\Omega} = (\boldsymbol{r} - \boldsymbol{r}')/R$, $\overline{\Sigma R} = \int_0^R \Sigma(s, E) ds$ is the optical distance between point $\boldsymbol{r}$ and $\boldsymbol{r}'$, $\Sigma_s(\boldsymbol{r}', \overline{\Omega}' \to \overline{\Omega}, E' \to E)$ is the

scattering kernel at point ***r***' from direction $\overline{\Omega}'$ at energy *E*' to direction $\overline{\Omega}$ with energy *E*, and $S(\boldsymbol{r}',\overline{\Omega},E)$ is the neutron source at point ***r***' of direction $\overline{\Omega}$ with energy *E*. In the above equation, while the fission neutron source is not expressed explicitly, it may be included in the source term.

Here, we assume that the scattering and the source are isotropic;

$$\Sigma_s(\boldsymbol{r},\overline{\Omega}'\to\overline{\Omega},E'\to E)=\frac{1}{4\pi}\Sigma_s(\boldsymbol{r},E'\to E) \quad , \tag{7.1-2a}$$

$$S(\boldsymbol{r},\overline{\Omega},E)=\frac{1}{4\pi}S(\boldsymbol{r},E) \tag{7.1-2b}$$

Integrating Eq.(7.1-1) over the whole angle of $\overline{\Omega}$, we obtain,

$$\varphi(\boldsymbol{r},E)=\int_{4\pi}d\overline{\Omega}\frac{1}{4\pi}\int_0^\infty dR\exp(-\overline{\Sigma R})\left[\int_0^\infty dE'\Sigma_s(\boldsymbol{r}',E'\to E)\varphi(\boldsymbol{r}',E')+S(\boldsymbol{r}',E)\right] \quad , \tag{7.1-3}$$

where $\varphi(\boldsymbol{r},E)$ is the neutron flux at point ***r*** with *E*, and is defined by

$$\varphi(r,E)=\int_{4\pi}d\overline{\Omega}\,\varphi(r,\overline{\Omega},E) \tag{7.1-4}$$

Equation (7.1-3) can be rewritten by the relation $d\boldsymbol{r}'=R^2dRd\overline{\Omega}$

$$\Sigma(\boldsymbol{r},E)\varphi(\boldsymbol{r},E)=\int d\boldsymbol{r}'\,P(\boldsymbol{r}'\to\boldsymbol{r},E)\left[\int_0^\infty dE'\Sigma_s(\boldsymbol{r}',E'\to E)\varphi(\boldsymbol{r}',E')+S(\boldsymbol{r}',E)\right] \quad , \tag{7.1-5}$$

where

$$P(\boldsymbol{r}'\to\boldsymbol{r},E)=\frac{\Sigma(\boldsymbol{r})}{4\pi R^2}\exp\left(-\int_0^R\Sigma_s(s)ds\right) \tag{7.1-6}$$

By the form of Eq.(7.1-6), the reciprocity relation holds,

$$\Sigma(\boldsymbol{r}',E)P(\boldsymbol{r}'\to\boldsymbol{r},E)=\Sigma(\boldsymbol{r},E)P(\boldsymbol{r}\to\boldsymbol{r}',E) \tag{7.1-7}$$

We divide the whole system under consideration into several regions. Each region is assumed homogeneous with respect to its nuclear properties, but different regions are not necessarily of different materials. The region is the spatial variable in the collision probability method. We denote space dependent cross sections with subscript *i* which are associated to the region *i*. Integrating Eq.(7.1-5) over V_j, we obtain

$$\Sigma_j(E)\int_{V_j}\varphi(\boldsymbol{r},E)d\boldsymbol{r}=\sum_i\int_{V_j}d\boldsymbol{r}\int_{V_i}d\boldsymbol{r}'\left[\int_0^\infty\Sigma_s(\boldsymbol{r}',E'\to E)\varphi(\boldsymbol{r}',E')dE'+S(\boldsymbol{r}',E)\right]\cdot P(\boldsymbol{r}'\to\boldsymbol{r},E)\,. \tag{7.1-8}$$

We make the flat flux approximation so that the neutron flux $\varphi(\boldsymbol{r},E)$ is assumed constant in

each region, for example, it is expressed by $\varphi_i(E)$ in the region *i*. This assumption leads the equation,

$$\Sigma_j(E)V_j\varphi_j(E) = \sum_i P_{ij}(E)V_i\left[\int_0^\infty \Sigma_{si}(E'\to E)\varphi_i(E)dE' + S_i(E)\right] \tag{7.1-9}$$

where the collision probability $P_{ij}(E)$ is defined by

$$P_{ij}(E) = \frac{\Sigma_j(E)}{4\pi V_i}\int_{V_j}d\boldsymbol{r}\int_{V_i}d\boldsymbol{r}'\frac{\exp(-\overline{\Sigma R})}{R^2} \tag{7.1-10}$$

It is explained as the probability that a neutron emitted uniformly and isotropically in the region *i* has its next collision in the region *j*. We divide the neutron energy range into multi-groups. The average flux in the energy interval ΔE_g is denoted by φ_{ig}. Then from Eq.(7.1-9), we obtain the simultaneous equation,

$$\Delta E_g\Sigma_{jg}V_j\varphi_{jg} = \sum_i P_{ijg}V_i\left[\sum_{g'}\Delta E_{g'}\Sigma_{sig'\to g}\varphi_{ig'} + \Delta E_g S_{ig}\right] \tag{7.1-11}$$

where ΔE_g and $\Delta E_{g'}$ are the energy width of the group *g* and *g'* and $\Sigma_{sig'\to g}$ is the scattering cross-section in the region *i* from the group *g'* to *g*, and is defined by

$$\Sigma_{sig'\to g} = \int_{\Delta Eg'}dE'\int_{\Delta Eg}dE\,\Sigma_{si}(E'\to E)\varphi_i(E') \Big/ \int_{\Delta Eg'}dE'\varphi_i(E') \tag{7.1-12}$$

As seen in the above derivation, once we obtain the collision probabilities, the neutron flux can be easily obtained by solving the simultaneous equation Eq.(7.1-11) by means of a matrix inversion or an iterative process.

Now we focus our considerations on the collision probability. The definition of the collision probability Eq.(7.1-10) can be expressed equivalently by

$$P_{ij} = \frac{1}{4\pi V_i}\int_{V_i}d\boldsymbol{r}\int_{4\pi}d\overline{\Omega}\int_{R_{j-}}^{R_{j+}}dR\Sigma_j\exp\left(-\int_0^R\Sigma(s)ds\right) \tag{7.1-13}$$

where the subscript to indicate the energy group is, hereafter, dropped for simplicity, and R_{j-} and R_{j+} denote the distances from point $\boldsymbol{r}$ to the inner and outer boundaries of the region *j* along the line through the points $\boldsymbol{r}$ and $\boldsymbol{r}'$.

From the form of Eq.(7.1-10), it can be seen easily that the reciprocity relation holds,

$$P_{ji}\Sigma_j V_j \quad = \quad P_{ij}\Sigma_i V_i \tag{7.1-14}$$

This relation is, as shown later, utilized to reduce the angular range of numerical integration.

The integration by R between R_{j-} and R_{j+} in Eq.(7.1-13) can be performed analytically in the homogeneous region j,

$$\int_{R_{j-}}^{R_{j+}} dR\Sigma_j \exp(-\overline{\Sigma R}) = \exp(-\overline{\Sigma R}_{j-}) \times \left\{1 - \exp\left(-\Sigma_j (R_{j+} - R_{j-})\right)\right\}$$
$$= \exp(-\overline{\Sigma R})_{R=R_{j-}} - \exp(-\overline{\Sigma R})_{R=R_{j+}}$$

The summation over j along the direction $\overline{\Omega}$ leaves only the first term of $\exp(-\overline{\Sigma R})_{R=0} = 1$, then the conservation law is easily shown as,

$$\sum_j P_{ij} = \frac{1}{4\pi V_i} \int_{V_i} d\boldsymbol{r} \int_{4\pi} d\overline{\Omega} = 1 \tag{7.1-15}$$

Similarly, the directional probabilities P_{ijk} defined by Benoist[25] which is used to provide the Behrens term of the anisotropic diffusion coefficients is expressed by

$$P_{ijk} = \frac{1}{4\pi V_i} \int_{V_i} d\boldsymbol{r} \int_{4\pi} d\overline{\Omega} 3\Omega_k^2 \int_{R_{j-}}^{R_{j+}} dR\Sigma_j \exp\left(-\int_0^R \Sigma(s)ds\right), \tag{7.1-16}$$

where k stands for direction, for example the parallel or perpendicular to the boundary plane in the case of plane lattice, and Ω_k denotes the directional cosine of $\overline{\Omega}$ in the direction k. The following relation holds:

$$\sum_k \Omega_k^2 = 1 \ , \tag{7.1-17}$$

The extension to include surfaces given by Beardwood[43] is as follows: If S is any surface (not necessarily closed) such that no line drawn outwards from a surface point $\overline{S}$ crosses S more once,

$$P_{is} = \frac{1}{4\pi V_i} \int_{V_i} d\boldsymbol{r} \int d\overline{S} \frac{\left(\boldsymbol{r} - \overline{S}\right)}{R_s{}^3} \exp\left(-\int_0^{R_s} \Sigma(s)ds\right) \tag{7.1-18}$$

is the probability that a neutron emitted from the region i crosses the outer boundary S, or an alternative expression,

$$P_{is} = \frac{1}{4\pi V_i} \int_{V_i} d\boldsymbol{r} \int_{4\pi} d\overline{\Omega} \exp\left(-\int_0^{R_s} \Sigma(s)ds\right) \tag{7.1-19}$$

is given, where R_s is a distance from the emitting point $\boldsymbol{r}$ to the surface point $\overline{S}$.

The isotropic reflective boundary condition is frequently used for the lattice cell calculation not only in the collision probability method but also in the Sn calculation. We shall describe its physical meaning and the application in the collision probability method using the explanation given by Bonalumi[48].

We assume the system with neither source nor absorption where the neutron flux distribution is uniform and isotropic everywhere. Then we suppose a cell in the entire space surrounded by a surface S is divided into N regions. We consider the balance of the collision rate in the region i

$$\Sigma_i \varphi V_i = \frac{\varphi}{4} S G_i + \sum_{j=1}^{N} P_{ji} \Sigma_i \varphi V_j \quad , \tag{7.1-20}$$

where the subscript i denotes that the quantity is assigned to the region i; and

Σ_i ; total macroscopic cross section,

φ ; uniform scalar flux,

V_i ; volume,

S ; area of the surface,

G_i ; probability that a neutron impinging on the surface has its first collision in the region i,

P_{ji} ; probability that a neutron emitted in the region j has its first collision in the region i.

The term on the left hand side (L.H.S.) denotes the collision rate in the region i. The first term on the right hand side (R.H.S.) denotes the contribution from the outside of the surface and the second term the contribution of the emission in each region inside of the surface. Using the reciprocity theorem Eq.(7.1-14) and the conservation theorem;

$$\sum_{j=1}^{N} P_{ij} \quad + \quad P_{is} \quad = \quad 1 \tag{7.1-21}$$

where P_{is} is the probability that a neutron emitted in the region i escapes from the outer surface S without suffering any collision, we have

$$G_i \quad = \quad \frac{4V_i}{S} \Sigma_i P_{is} \tag{7.1-22}$$

Then we define G_s as the probability that a neutron impinging from the outer surface into the inside of the surface escapes from the surface without suffering any collision:

$$G_s \quad = \quad 1 - \sum_{i=1}^{N} G_i \tag{7.1-23}$$

When the cells are set in an array, we get the collision probabilities for the lattice cell by using the quantities for the isolated cell as follows:

$$P_{ij}(lattice) = P_{ij}(isolated) + P_{is} G_j + P_{is} G_s G_j + P_{is} G_s{}^2 G_j + ... ,$$

which can be rewritten as

$$P_{ij}(lattice) = P_{ij}(isolated) + P_{is}\frac{G_j}{1-G_s}. \tag{7.1-24}$$

7.1.2 Collision Probabilities for Slab Lattice

In a one-dimensional slab geometry shown in Fig.7.1-1, we have

$R = \left|\frac{x'-x}{\cos\theta}\right|$,

$d\boldsymbol{r} = dx$,

$d\Omega = 2\pi \sin\theta d\theta$

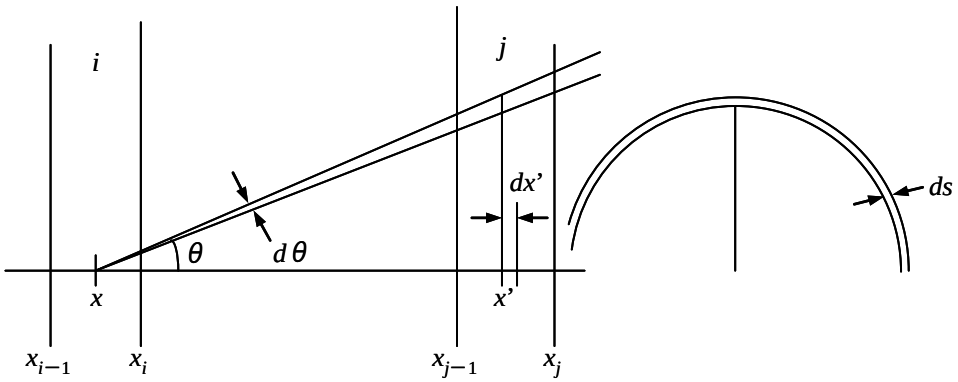


Fig.7.1-1 Coordinates in slab geometry

We assume that the system is divided into an array of slabs. The slab *i* has its left edge at x_{i-1} and its total cross section denoted by Σ_i. Then we have

$$P_{ij} = \frac{1}{2(x_i - x_{i-1})}\int_{x_{i-1}}^{x_i} dx \int_{x_{j-1}}^{x_j} dx' \int_0^{\pi/2} \Sigma(x')\frac{\sin\theta}{\cos\theta}\cdot \exp\left\{-\int_x^{x'} \Sigma(t)dt / \cos\theta\right\} d\theta \tag{7.1-25}$$

for the case $x_i < x_j$-1, and the optical distance which appears in the exponential term in Eq.(7.1-25) is reduced to

$$\int_x^{x'} \Sigma(t)dt = \Sigma_i(x_i - x) + \Sigma_j(x'-x_{j-1}) + \sum_{k=i+1}^{j-1}\lambda_k$$

where $\lambda_k = \Sigma_k(x_k - x_{k-1})$.

Then we can carry out the integration over *x* and *x*', and we get

$$P_{ij} = \frac{1}{2\lambda_i}\int_0^{\pi/2} \sin\theta\cos\theta\, d\theta \left\{1-\exp\left(-\frac{\lambda_i}{\cos\theta}\right)\right\}\cdot\left\{1-\exp\left(-\frac{\lambda_j}{\cos\theta}\right)\right\}\cdot\exp\left\{-\sum_{k=i+1}^{j-1}\frac{\lambda_k}{\cos\theta}\right\}$$

Now we introduce the exponential integral function, E_{in} defined by Schloemich[49)]

$$E_{in}(x) = \int_0^1 d\mu\ \mu^{n-1}\exp\left(-\frac{x}{\mu}\right)$$

We have the final form of P_{ij} for the case $x_i < x_j$ as follows:

$$P_{ij} = \frac{1}{2\lambda_i}\left\{E_{i3}(\lambda_{ij}) - E_{i3}(\lambda_{ij}+\lambda_i) - E_{i3}(\lambda_{ij}+\lambda_j) + E_{i3}(\lambda_{ij}+\lambda_i+\lambda_j)\right\} \tag{7.1-26}$$

where $\lambda_{ij} = \sum_{k=i+1}^{j-1}\lambda_k$, for $x_i<x_j$ (7.1-27)

Equation (7.1-26) is identical with the formulation derived by Honeck[34)] started by the plane transport kernel expressed by the E_{i1} function.

Next we shall consider the case where $x_i > x_j$, the optical distance is reduced to

$$\int_x^{x'}\Sigma(t)dt = \Sigma_i(x-x_{i-1}) + \Sigma_j(x_j - x') + \sum_{k=j+1}^{i-1}\lambda_k$$

by using the same procedure as $x_i<x_j$ we get the same expression as Eq.(7.1-26) except for the definition of λ_{ij}. In this case we have

$$\lambda_{ij} = \sum_{k=j+1}^{i-1}\lambda_k \quad , \quad \text{for } x_i > x_j \tag{7.1-28}$$

In the last case where $x_i = x_j$, the optical distance in Eq.(7.1-25) is reduced to

$$\left|\int_x^{x'}\Sigma(t)dt\right| = \begin{cases}\Sigma_i(x'-x) & \text{for } x' > x \\ \Sigma_i(x-x') & \text{for } x > x'\end{cases}$$

Integrating over x and x' gives the final form of P_{ii} by

$$P_{ii} = 1 - \frac{1}{\lambda_i}\left\{E_{i3}(0) - E_{i3}(\lambda_i)\right\} \tag{7.1-29}$$

If the λ_i's are so small that the differences in Eq.(7.1-26) and in Eq.(7.1-29) can not be obtained accurately in the numerical calculation, we should use the following differential forms instead of Eqs.(7.1-26) and (7.1-29), respectively,

$$P_{ij} = \frac{\lambda_j}{2}E_{i1}(\lambda_{ij} + \lambda_i/2 + \lambda_j/2) \quad , \tag{7.1-30}$$

$$P_{ii} = \lambda_i E_{i1}(\lambda_i/2) \tag{7.1-31}$$

We, however, should take care of the property of the E_{i1} function which has the logarithmic singularity.

We consider now the lattice cell system where a unit cell is divided into N regions and the collision region j lies periodically. A sum of such terms as Eq.(7.1-26) gives

$$P_{ij} = \frac{1}{2\lambda_i}\sum_{l=0}\Big\{E_{i3}(\lambda_{ij}^{l1}) - E_{i3}(\lambda_{ij}^{l1}+\lambda_i) - E_{i3}(\lambda_{ij}^{l1}+\lambda_j) + E_{i3}(\lambda_{ij}^{l1}+\lambda_i+\lambda_j) + E_{i3}(\lambda_{ij}^{l2}) - E_{i3}(\lambda_{ij}^{l2}+\lambda_i) - E_{i3}(\lambda_{ij}^{l2}+\lambda_j) + E_{i3}(\lambda_{ij}^{l2}+\lambda_i+\lambda_j)\Big\} \tag{7.1-32}$$

where

$$\begin{aligned}\lambda_{ij}^{l1} &= \sum_{k=i+1}^{j-1}\lambda_k + l\times\sum_{k=1}^{N}\lambda_k \\ \lambda_{ij}^{l2} &= \sum_{k=1}^{i-1}\lambda_k + \sum_{k=j+1}^{N}\lambda_k + \sum_{k=1}^{i-1}\lambda_k + l\times\sum_{k=1}^{N}\lambda_k\end{aligned} \tag{7.1-33}$$

The summation over l is achieved separately by λ_{ij}^{l1} or λ_{ij}^{l2} series until λ_{ij}^{l1} or λ_{ij}^{l2} exceeds the fixed optical length, say, 6, respectively. For the case where $j<i$, i and j in Eq.(7.1-33) must be replaced by j and i, respectively.

For the case $i = j$ we have

$$P_{ii} = 1 - \frac{1}{\lambda_i}\{E_{i3}(0) - E_{i3}(\lambda_i)\} + \frac{1}{\lambda_i}\sum_{l=0}\Big\{E_{i3}(\lambda_{ii}^{l}) - 2E_{i3}(\lambda^{l}{}_{ii}+\lambda_i)) + E_{i3}(\lambda^{l}{}_{ii}+2\lambda_i)\Big\} \tag{7.1-34}$$

where $$\lambda_{ii}^{l} = (l+1)\times\sum_{k=1}^{N}\lambda_k - \lambda_i \tag{7.1-35}$$

When the lattice cell is arranged symmetrically, we may reduce the computing time into half using the reciprocity relation, while it is not utilized in the SRAC code.

Now we consider the explicit form of the directional probabilities. For the perpendicular direction to the boundary plane, we have $3\cos^2\theta$ as $3\Omega_\perp^2$ c.f. Fig.7.1-1, by which the integrand in Eq.(7.1-25) has to be multiplied. The similar procedure gives us the expression of $P_{ij\perp}$ corresponding to Eq.(7.1-26) as follows:

$$P_{ij\perp} = \frac{3}{2\lambda_i}\Big\{E_{i5}(\lambda_{ij}) - E_{i5}(\lambda_{ij}+\lambda_i) - E_{i5}(\lambda_{ij}+\lambda_j) + E_{i5}(\lambda_{ij}+\lambda_i+\lambda_j)\Big\}, \tag{7.1-36}$$

and corresponding to Eq.(7.1.29)

$$P_{ii\perp} = 1 - \frac{3}{2\lambda_i}\{E_{i5}(0) - E_{i5}(\lambda_i)\} \tag{7.1-37}$$

For the parallel direction we can easily obtain the explicit form, but it is not necessary because the following relation holds:

$$P_{ij} = \frac{1}{3} P_{ij\perp} + \frac{2}{3} P_{ij//} \tag{7.1-38}$$

The relation is derived from

$$1 = \sum_k \Omega^2{}_k = \Omega^2{}_\perp + 2\Omega^2_{//}$$

So we can obtain $P_{ij//}$ by subtraction.

At the end of this section we show the expression for the escape probability P_{is}:

$$P_{is} = \frac{1}{2\lambda_i} \left\{ E_{i3}(\lambda^1_{is}) - E_{i3}(\lambda^1_{is} + \lambda_i) + E_{i3}(\lambda^2_{is}) - E_{i3}(\lambda^2_{is} + \lambda_i) \right\} \tag{7.1-39}$$

where $\lambda^1_{is} = \sum_{k=1}^{i-1} \lambda_k$, $\lambda^2_{is} = \sum_{k=i+1}^{N} \lambda_k$.

7.1.3 Collision Probabilities for One-dimensional Cylindrical Lattice

We consider the infinitely long cylinder which is divided into several annular shells. The outer radius of the shell i is r_i. We suppose that a neutron emitted at the point P in the shell i has its first collision at the point Q in the shell j. The position of P is defined by only the distance from the cylindrical axis; r. The line PQ makes an angle θ with the vertical line. We define the point Q' as the projection of the point Q on the horizontal cross-section so that the line PQ' makes an angle θ with the line PO.

The distance between P and Q' is R. In the cylindrical coordinate system as shown in Fig.7.1-2a, we have the collision probability P_{ij} as,

$$P_{ij} = \frac{2}{V_i} \int_{r_{i-1}}^{r_i} r dr \int_0^{\pi} d\beta \int_0^{\pi/2} \sin\theta \, d\theta \int_{R_{j-}}^{R_{j+}} dR \frac{\Sigma_j}{\sin\theta} \exp\left\{ - \int_0^R \frac{\Sigma(s)}{\sin\theta} ds \right\} , \tag{7.1-40}$$

where

$$V_i = \pi(r_i^2 - r_{i-1}^2) \tag{7.1-41}$$

Then we transform the variables r, β and R into new ones ρ, x and x' as illustrated in Fig.7.1-2b. We define the perpendicular distance OM from O to the line PQ' by ρ, the distance between P and M by x, and the distance between Q' and M by x'. There are three relations among variables:

$$r^2 = \rho^2 + x^2$$
$$r\sin\beta = \rho \qquad (7.1\text{-}42)$$
$$R = x - x'$$

Using these relations we have the Jacobian

$$\frac{\partial(r,\beta,R)}{\partial(\rho,x,x')} = \frac{1}{r} \qquad (7.1\text{-}43)$$

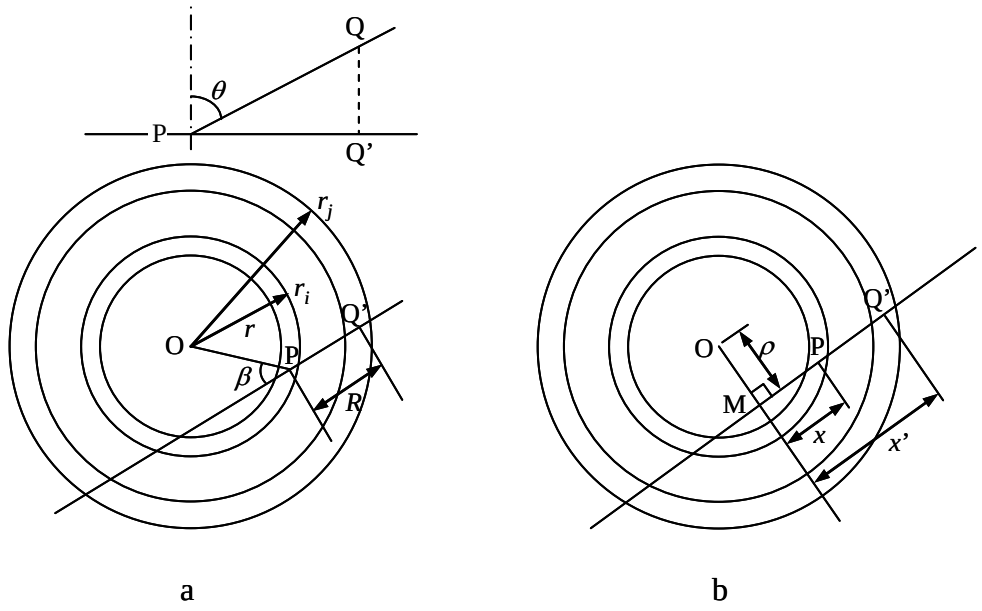


Fig.7.1-2 Cylindrical coordinates

Then we can rewrite Eq.(7.1-40) using new variables by

$$P_{ij} = \frac{2}{V_i}\int_0^{r_i} dr \int_0^{\pi/2} d\theta \int_{x_{i-1}}^{x_i} dx \int_{x'_{j-1}}^{x'_j} dx' \Sigma_j \left[\exp\left\{ -\left| \int_x^{x'} \Sigma(t)dt \right| / \sin\theta \right\} + \exp\left\{ -\left| \int_{-x}^{x'} \Sigma(t)dt \right| / \sin\theta \right\} \right] \qquad (7.1\text{-}44)$$

where

$$x_i = \sqrt{r_i^2 - \rho^2} \quad \text{for} \quad r_i > \rho$$
$$x_i = 0 \quad \text{for} \quad r_i < \rho$$

and Σ_i denotes the total macroscopic cross-section of the shell *i*.

For the case $r_j > r_i$, the optical distances which appear in the exponential terms in Eq.(7.1-44)

are reduced to

$$\int_x^{x'} \Sigma(t)dt = \Sigma_i (x_i - x) + \Sigma_j (x' - x_{j-1}) + \sum_{k=i+1}^{j-1} \lambda_k \quad ,$$

$$\int_{-x}^{x'} \Sigma(t)dt = \Sigma_i (x - x_{i-1}) + \Sigma_j (x' - x_{j-1}) + \sum_{k=i+1}^{j-1} \lambda_k + 2\sum_{k=1}^{i-1} \lambda_k + \lambda_i$$

$$= \Sigma_i (x - x_{i-1}) + \Sigma_j (x' - x_{j-1}) + \sum_{k=1}^{j-1} \lambda_k + \sum_{k=1}^{i-1} \lambda_k ,$$

where $\lambda_k = \Sigma_k (x_k - x_{k-1})$.

Then we can carry out the integration over x and x', and we get

$$P_{ij} = \frac{2}{\Sigma_i V_i} \int_0^{r_i} d\rho \int_0^{\pi/2} \sin\theta d\theta \left\{ 1 - \exp\left(-\frac{\lambda_i}{\sin\theta} \right) \right\} \left\{ 1 - \exp\left(-\frac{\lambda_j}{\sin\theta} \right) \right\}$$
$$\times \left\{ \exp\left(-\sum_{k=1}^{i-1} \lambda_k / \sin\theta - \sum_{k=1}^{j-1} \lambda_k / \sin\theta \right) \right\} \quad .$$

Now we introduce the Bickley-Naylor function[50)]

$$K_{in}(x) = \int_0^{\pi/2} d\theta \sin^{n-1}\theta \exp\left(-\frac{x}{\sin\theta} \right) \tag{7.1-45}$$

We have the final form of P_{ij} for the case $r_i < r_j$, as follows:

$$P_{ij} = \frac{2}{\Sigma_i V_i} \int_0^{r_i} d\rho \Big\{ K_{i3}(\lambda_{ij}^1) - K_{i3}(\lambda_{ij}^1 + \lambda_i) - K_{i3}(\lambda_{ij}^1 + \lambda_j) + K_{i3}(\lambda_{ij}^1 + \lambda_i + \lambda_j)$$
$$+ K_{i3}(\lambda_{ij}^2) - K_{i3}(\lambda_{ij}^2 + \lambda_i) - K_{i3}(\lambda_{ij}^2 + \lambda_j) + K_{i3}(\lambda_{ij}^2 + \lambda_i + \lambda_j) \Big\} \tag{7.1-46}$$

where

$$\lambda_{ij}^1 = \sum_{k=i+1}^{j-1} \lambda_k \quad ,$$
$$\lambda_{ij}^2 = \sum_{k=1}^{i-1} \lambda_k + \sum_{k=1}^{j-1} \lambda_k \qquad \text{for} \quad r_i < r_j \tag{7.1-47}$$

Next we consider P_{ij} for the case $r_i > r_j$, where the optical distances differ from the case $r_i < r_j$ because Q is located inside of P so that $x' < x$. In this sense the symbol of the absolute value is required. We rewrite locally the optical distance as follows:

$$\left| \int_x^{x'} \Sigma(t)dt \right| = \int_{x'}^{x} \Sigma_i(t)dt = \Sigma_j (x_j - x') + \Sigma_i (x - x_{i-1}) + \sum_{k=j+1}^{i-1} \lambda_k \quad .$$

Integration over x and x' gives the final form of P_{ij} for the case $r_i > r_j$, which is exactly the same expression as in Eq.(7.1-46) but λ_{ij}^1 in Eq.(7.1-47) must be replaced by

$$\lambda_{ij}^{1} \quad = \quad \sum_{k=j+1}^{i-1} \lambda_k \qquad \text{for} \quad r_i > r_j \tag{7.1-48}$$

We have not yet considered the case where the shell *i* coincides with the shell *j*. In this case the optical distances are reduced to

$$\left| \int_{x}^{x'} \Sigma(t)dt \right| \quad = \quad \begin{cases} \Sigma_i (x' - x) & \text{for} \quad x' > x\,, \\ \Sigma_i (x - x') & \text{for} \quad x > x'\,, \end{cases}$$

$$\int_{-x}^{x'} \Sigma(t)dt \quad = \quad \Sigma_i (x' - x_i) + \Sigma_i (x - x_{i-1}) + 2\sum_{k=1}^{i-1} \lambda_k \quad .$$

In the integration over *x*' for the first term on R.H.S. of Eq.(7.1-44), we must divide the range into (x_{i-1}, x) and (x, x_i) and then we have

$$\begin{aligned} P_{ii} = \frac{2}{\Sigma_i V_i} \int_0^{r_{i-1}} d\rho \int_0^{\pi/2} d\theta \Bigg[& 2\lambda_i \sin\theta - 2\sin^2\theta \left\{ 1 - \exp\left(-\frac{\lambda_i}{\sin\theta} \right) \right\} \\ & + \left\{ 1 - \exp\left(-\frac{\lambda_i}{\sin\theta} \right) \right\}^2 \sin^2\theta \exp\left(-2\sum_{k=1}^{i-1} \frac{\lambda_k}{\sin\theta} \right) \Bigg] \\ & + \frac{2}{\Sigma_i V_i} \int_{r_{i-1}}^{r_i} d\rho \int_0^{\pi/2} d\theta \left[2\lambda_i \sin\theta - \sin^2\theta \left\{ 1 - \exp\left(-2\frac{\lambda_i}{\sin\theta} \right) \right\} \right] \end{aligned}$$

Using the K_{in} function we get the final form of P_{ii} as follows:

$$\begin{aligned} P_{ii} = & \frac{2}{\Sigma_i V_i} \int_0^{r_{i-1}} d\rho \left\{ 2\lambda_i - 2K_{i3}(0) + 2K_{i3}(\lambda_i) + K_{i3}(\lambda_{ii}) - 2K_{i3}(\lambda_{ii} + \lambda_i) + K_{i3}(\lambda_{ii} + 2\lambda_i) \right\} \\ & + \frac{2}{\Sigma_i V_i} \int_{r_{i-1}}^{r_i} d\rho \left\{ 2\lambda_i - K_{i3}(0) + K_{i3}(2\lambda_i) \right\} \end{aligned} \tag{7.1-49}$$

where

$$\lambda_{ii} = 2\sum_{k=1}^{i-1} \lambda_k \tag{7.1-50}$$

If the λ_i's are so small that the differences in the brackets of Eq.(7.1-46) and (7.1-49) can not be obtained accurately in numerical calculation, we should use instead of Eqs.(7.1-46) and (7.1-49), the following differential forms:

$$P_{ij} = \frac{2}{\Sigma_i V_i} \int_0^{r_i} d\rho \lambda_i \lambda_j \left\{ K_{i1}(\lambda_{ij}^1) + K_{i1}(\lambda_{ij}^2) \right\} \tag{7.1-51}$$

$$P_{ii} = \frac{1}{\Sigma_i V_i} \int_0^{r_{i-1}} d\rho \left\{ \lambda_i^2 K_{i1}(\lambda_i / 2) + \lambda_i^2 K_{i1}(\lambda_{ii}) \right\} \tag{7.1-52}$$

If we assume the cylindricalized cell with the perfect reflective outer boundary, more terms like those in Eq.(7.1-46) are required as follows;

$$
\begin{aligned}
& K_{i3}(\lambda_{ij}^3) - K_{i3}(\lambda_{ij}^3 + \lambda_i) - K_{i3}(\lambda_{ij}^3 + \lambda_j) + K_{i3}(\lambda_{ij}^3 + \lambda_i + \lambda_j) \\
& + K_{i3}(\lambda_{ij}^4) - K_{i3}(\lambda_{ij}^4 + \lambda_i) - K_{i3}(\lambda_{ij}^4 + \lambda_j) + K_{i3}(\lambda_{ij}^4 + \lambda_i + \lambda_j) \\
& + \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
& + K_{i3}(\lambda_{ij}^n) - K_{i3}(\lambda_{ij}^n + \lambda_i) - K_{i3}(\lambda_{ij}^n + \lambda_j) + K_{i3}(\lambda_{ij}^n + \lambda_i + \lambda_j) \\
& + \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots
\end{aligned}
$$

where

$$
\begin{aligned}
& \lambda_{ij}^3 = \lambda_{ij}^1 + \lambda_j + 2\sum_{k=i+1}^{N} \lambda_k \quad , \\
& \lambda_{ij}^4 = \lambda_{ij}^2 + \lambda_j + 2\sum_{k=i+1}^{N} \lambda_k \quad , \\
& \cdots\cdots\cdots\cdots\cdots\cdots\cdots \quad , \\
& \lambda_{ij}^n = \lambda_{ij}^{n-2} + \lambda_j + 2\sum_{k=i+1}^{N} \lambda_k \ ,
\end{aligned}
$$

These terms to be used in the integrand of Eq.(7.1-46) are the generalized form of those appearing in the expression of $P_{1\to 2}$ given by Takahashi[35)], while the integration variable has not yet been transformed to ρ.

As regards the directional probabilities in the cylindrical coordinates, we know for the axial direction $3\Omega_z^2 = 3\cos^2\theta$ and for the radial direction $3\Omega_r^2 = (3/2)\sin^2\theta$. For the latter, P_{ijr} is obtained by multiplying the integrand in Eq.(7.1-40) by $(3/2)\sin^2\theta$. It is not worth while to repeat here the whole expressions for each condition. It is enough for us to know only the fact that all the terms expressed by $K_{in}(x)$ must be replaced by $(3/2)K_{i\ (n+2)}(x)$. Similarly to the slab system, the following relation holds:

$$
P_{ij} \quad = \quad \frac{1}{3} P_{ijz} \quad + \quad \frac{2}{3} P_{ijr} \tag{7.1-53}
$$

We know that the isotropic boundary condition brings more accurate result and is less time-consuming than the perfect reflective boundary condition to evaluate the flux distribution in the real cell by the cylindricalized model. In this case the probability, P_{is} that a neutron emitted in the shell i escapes from the outer boundary without suffering any collision is required. It is easily obtained as

$$
P_{is} = \frac{2}{\Sigma_i V_i} \int_0^{r_i} d\rho \left\{ K_{i3}(\lambda_{is}^1) - K_{i3}(\lambda_{is}^1 + \lambda_i) + K_{i3}(\lambda_{is}^2) - K_{i3}(\lambda_{is}^2 + \lambda_i) \right\}, \tag{7.1-54}
$$

where

$$\begin{aligned} \lambda_{is}^{1} &= \sum_{k=i+1}^{N} \lambda_k \quad , \\ \lambda_{is}^{2} &= \sum_{k=1}^{i-1} \lambda_k + \sum_{k=1}^{N} \lambda_k \quad . \end{aligned} \tag{7.1-55}$$

7.1.4 Collision Probabilities for Spherical System

A spherical system is divided into N spherical shells. We define the shell i that is bounded by two spherical surfaces of radii r_{i-1} and r_i. The shells are numbered by increasing order of r_i. In general, a probability P_{ij} that a neutron emitted in the region i has its first collision in the region j is defined as

$$P_{ij} = \frac{1}{4\pi V_i} \int_{V_i} dV \int_{4\pi} d\overline{\Omega} \int_{R \subset V_j} dR \Sigma_j \exp\left\{ - \int_0^R \Sigma(s) ds \right\} \tag{7.1-56}$$

The integrand on R.H.S. of Eq.(7.1-56) is interpreted as follows by referring Fig.7.1-3a. A neutron emitted at a point P in the region i moves toward a point Q which is in distance R from the point P, has the exponential decay by the optical length $\int_0^R \Sigma(s) ds$ and suffers its collision at the layer of thickness dR in region j of the cross-section Σ_j. In the spherically symmetric system the position of the point P is defined only by the distance r from the center of the system, C. The position of the point Q is defined by the distance R from the point P, and the angle θ made by the lines PQ and PC (See Fig.7.1-3a). In this coordinate system,

$$\begin{aligned} dV &= 4\pi r^2 dr \qquad && 0 < r < r_N \ , \\ d\overline{\Omega} &= 2\pi \sin\theta d\theta \qquad && 0 \le \theta \le \pi \ , \end{aligned}$$

and Eq.(7.1-56) is rewritten by a triple integral form:

$$P_{ij} = \frac{4\pi \Sigma_j}{V_i} \int_0^{r_N} r^2 dr \int_0^{\pi} \sin\theta d\theta \int_{R \subset V_j} dR \exp\left\{ - \int_0^R \Sigma(s) ds \right\} \quad . \tag{7.1-57}$$

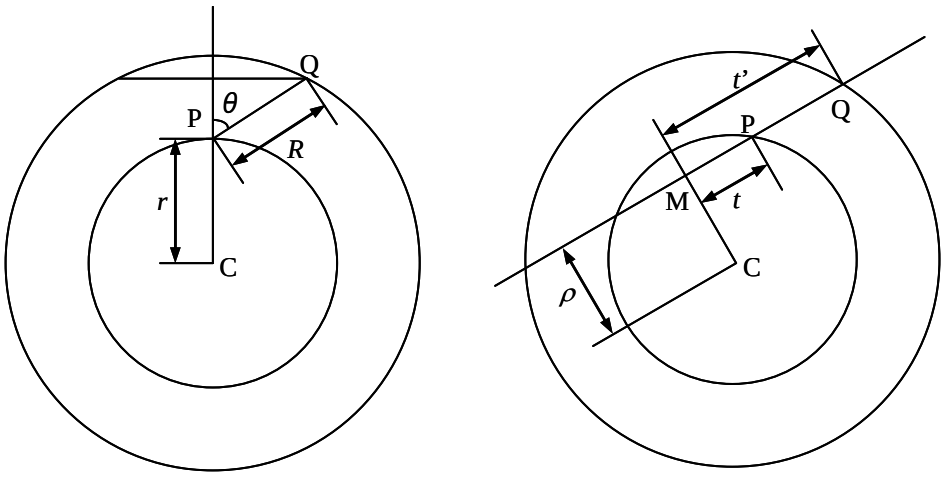


Fig.7.1-3 Spherical coordinates

To perform analytically the integration as far as possible, the coordinates shown in Fig.7.1-3a are transformed into the new coordinates shown in Fig.7.1-3b where the perpendicular length CM is ρ. The positions of points P and Q are defined by the distances t and t', respectively, from the point M. The following relations among variables are found:

$$\begin{aligned} & r^2 = t^2 + \rho^2 \quad , \\ & r\sin\theta = \rho \quad , \\ & R = t' - t \quad . \end{aligned} \tag{7.1-58}$$

The Jacobian is then obtained as follows:

$$\frac{\partial(r,\theta,R)}{\partial(\rho,t,t')} = -\frac{1}{r} \quad . \tag{7.1-59}$$

The probability is rewritten using the new variables by

$$P_{ij} = \frac{2\pi\Sigma_j}{V_i}\int_0^{r_N}\rho d\rho\int_{t\subset V_i} dt\int_{t'\subset V_j} dt'\exp\left\{-\int_0^{t-t'}\Sigma(s)ds\right\} \quad . \tag{7.1-60}$$

As the nuclear cross-section in each shell is uniform, we can integrate Eq.(7.1-60) over t and t'. Finally the shell-to-shell collision probabilities are given in the form of single integral (See Fig.7.1-4);

$$P_{ij} = \frac{2\pi}{\Sigma_i V_i}\int_0^{r_{i-1}} \rho d\rho\{1-\exp(-\lambda_i)\}\{1-\exp(-\lambda_j)\}$$
$$\times\left\{\exp\left(-\sum_{k=i+1}^{j-1}\lambda_k\right)+\exp\left(-2\sum_{k=1}^{i-1}\lambda_k-\lambda_i-\sum_{k=i+1}^{j-1}\lambda_k\right)\right\} \qquad \text{for } i<j \qquad (7.1\text{-}61)$$
$$+\frac{2\pi}{\Sigma_i V_i}\int_{r_{i-1}}^{r_i} \rho d\rho\{1-\exp(-2\lambda_i)\}\{1-\exp(-\lambda_j)\}\exp\left(-\sum_{k=i+1}^{j-1}\lambda_k\right)$$

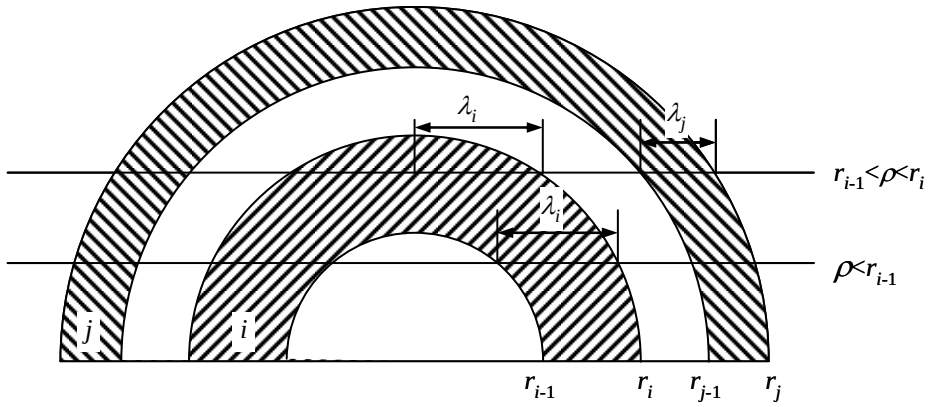


Fig.7.1-4 Neutron lines in case $i<j$

$$P_{ii} = \frac{2\pi}{\Sigma_i V_i}\int_0^{r_i-1} \rho d\rho\{\lambda_i-1+\exp(-\lambda_i)\}\{1-\exp(-\lambda_i)\}^2\exp\left(-2\sum_{k=1}^{i-1}\lambda_k\right) \qquad \text{for } i=j \qquad (7.1\text{-}62)$$
$$+\frac{2\pi}{\Sigma_i V_i}\int_{r_i-1}^{r_i} \rho d\rho\{2\lambda_i-1+\exp(-2\lambda_i)\}$$

where

$$t_i = \sqrt{r_i^2-\rho^2} \qquad for \quad r_i \geq \rho \quad ,$$
$$t_i = 0 \qquad for \quad r_i < \rho \qquad (7.1\text{-}63)$$

$$\lambda_i = \Sigma_i\,(t_i - t_{i-1}) \qquad (7.1\text{-}64)$$

For $i>j$, the similar expression to Eq.(7.1-61) can easily be obtained, but the reciprocity theorem gives P_{ji} directly from P_{ij}.

Now we have the escape probability P_{is} as

$$P_{is} = \frac{2\pi}{\Sigma_i V_i}\int_0^{r_{i-1}} \rho d\rho \{1-\exp(-\lambda_i)\}\cdot\exp\left(-\sum_{k=i+1}^{N}\lambda_k\right)\cdot\left\{1+\exp\left(-2\sum_{k=1}^{i-1}\lambda_k-\lambda_i\right)\right\}$$
$$+\frac{2\pi}{\Sigma_i V_i}\int_{r_{i-1}}^{r_i} \rho d\rho \{1-\exp(-2\lambda_i)\}\exp\left(-\sum_{k=i+1}^{N}\lambda_k\right) \quad (7.1\text{-}65)$$

In the SRAC code, the integrands in Eqs.(7.1-61) and (7.1-62) to possible pairs of (*i*, *j*) are, first calculated for a fixed ρ. Then, the integration over ρ is accomplished by changing the value of ρ.

7.1.5 Collision Probabilities for Two-dimensional Cylindrical Lattice

In the cylindrical system with general shape of its cross section and of infinite height, the collision probability from a region *i* to another region *j*, P_{ij}, is expressed by the following Eq.(7.1-66) in the coordinate system of Fig.7.1-5, assuming flat flux in each region and isotropic emission in the laboratory system;

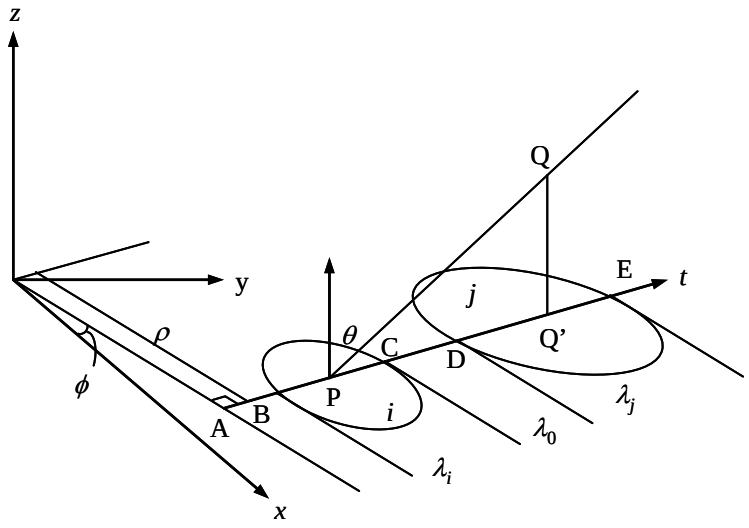


Fig.7.1-5 Cylindrical coordinate system

$$P_{ij} = \left[\int_{-\infty}^{+\infty}\rho d\rho\int_0^{2\pi}d\varphi\int_0^{\pi/2}\sin\theta d\theta\int_{AB}^{AC}dt\,\exp\left\{-\frac{\Sigma_i|AC-t|}{\sin\theta}\right\}\int_{AD}^{AE}dt'\frac{\Sigma_j}{\sin\theta}\right.$$
$$\left.\times exp\left\{-\frac{\Sigma_j|t'-AD|}{\sin\theta}\right\}\exp\left\{-\left|\int_{AC}^{AD}\Sigma(s)ds\right|\Big/\sin\theta\right\}\right] \quad (7.1\text{-}66)$$
$$\Big/\quad\left[\int_{-\infty}^{+\infty}\rho d\rho\int_0^{2\pi}d\varphi\int_0^{\pi/2}\sin\theta d\theta\int_{AB}^{AC}dt\right]$$

In Fig.7.1-5, the line PQ' defined by ρ and φ is the projection of the neutron line PQ on the horizontal plane. The points P and Q are, respectively, the source and collision positions. The point A is the origin of measures of *t*, *t*' and *s*. The points B, C, D and E are the points of intersection of the line PQ' with the region boundaries. A restriction on the moving direction of a neutron is imposed so that a neutron moves only to the positive direction of *t* along the line PQ'. If the line PQ' enters the region *j* more than once, a sum of Eq.(7.1-66) is required.

The self collision probability, P_{ii} is expressed by the following Eq.(7.1-67), where the point Q is in the region *i*.

$$P_{ii} = \left[\int_{-\infty}^{+\infty} \rho d\rho \int_0^{2\pi} d\varphi \int_0^{\pi/2} \sin\theta d\theta \int_{AB}^{AC} dt \int_t^{AC} dt' \frac{\Sigma_i}{\sin\theta} \exp\left\{ -\frac{\Sigma_i |t-t'|}{\sin\theta} \right\} \right] \Big/ \left[\int_{-\infty}^{+\infty} \rho d\rho \int_0^{2\pi} d\varphi \int_0^{\pi/2} \sin\theta d\theta \int_{AB}^{AC} dt \right] \tag{7.1-67}$$

If the line PQ' reenters the region *i*, a sum of such a term as Eq.(7.1-66) is also required for obtaining P_{ii}.

The six-fold integrals of Eqs.(7.1-66) and (7.1-67) are reduced to the double integrals as follows:

$$P_{ij} = \frac{1}{2\pi\Sigma_i V_i} \int_{-\infty}^{+\infty} d\rho \int_0^{2\pi} d\varphi \left\{ K_{i3}(\lambda_0) - K_{i3}(\lambda_0 + \lambda_i) - K_{i3}(\lambda_0 + \lambda_j) + K_{i3}(\lambda_0 + \lambda_i + \lambda_j) \right\}, \tag{7.1-68}$$

$$P_{ii} = \frac{1}{2\pi\Sigma_i V_i} \int_{-\infty}^{+\infty} d\rho \int_0^{2\pi} d\varphi \left\{ \lambda_i - K_{i3}(0) + K_{i3}(\lambda_i) \right\} \ , \tag{7.1-69}$$

where λ_i and λ_j denote the optical path lengths (the physical path multiplied by the macroscopic total cross section), λ_i =BC*Σ_i, λ_j =DE*Σ_j and λ_0 stands for the sum of optical path lengths between C and D; and K_{i3} is the third order Bickley-Naylor function.

The escape probability P_{is} defined as a neutron emitted in the region *i* escapes from the surface without suffering collision, is expressed as

$$P_{is} = \frac{1}{2\pi\Sigma_i V_i} \int_{-\infty}^{+\infty} d\rho \int_0^{2\pi} d\varphi \left\{ K_{i3}(\lambda_{is}) - K_{i3}(\lambda_{is} + \lambda_i) \right\} \ , \tag{7.1-70}$$

where λ_{is} is the optical path length along the line from the edge of the region *i* to the surface of the system.

As for the directional probabilities, similarly to the case of the one-dimensional cylinder, it is not necessary to write the whole components and hence a few samples are shown here:

$$P_{ijr} = \frac{3}{4\pi\Sigma_i V_i} \int_{-\infty}^{+\infty} d\rho \int_0^{2\pi} d\varphi \left\{ K_{i5}(\lambda_0) - K_{i5}(\lambda_0 + \lambda_i) - K_{i5}(\lambda_0 + \lambda_j) + K_{i5}(\lambda_0 + \lambda_i + \lambda_j) \right\} \tag{7.1-71}$$

$$P_{iir} = \frac{1}{4\pi\Sigma_i V_i}\int_{-\infty}^{+\infty} d\rho \int_0^{2\pi} d\varphi \{2\lambda_i - 3K_{i5}(0) + 3K_{i5}(\lambda_i)\} \tag{7.1-72}$$

Thus we have the double integration of the linear combination of K_{in} function as a final form of the collision probabilities for the two-dimensional cylindrical system.

7.1.6 Ray-Trace Method for Integration of Collision Probabilities

The integration by ρ and φ in Eqs.(7.1-66) and (7.1-67) is carried out by the trapezoidal integration formula with equal width and weight in a general two-dimensional geometry. As seen, a pair of ρ and φ determines a neutron line across the cell.

In one-dimensional geometries such as cylinder and sphere, no integration over the azimuthal angle φ is needed as the geometry is invariant about the azimuthal angle φ. In this case, the range of the integration over ρ ; (0, r_N) is sub-divided into N regions by r_i where r_i is the outer boundary of the i-th annular region, in order to perform an efficient Gaussian quadrature in each sub-division, so that we can avoid the singularity in the integrand. That is, the argument λ_i vanishes as ρ approaches r_i and this causes the integrand to have an undefined derivative at this point. The efficiency of the Gaussian quadrature is shown by an example that the 10-point Gaussian integration for $(r^2 - \rho^2)^{1/2}$ gives the area of a circle by an accuracy of 0.1%.

For the two-dimensional cell of complex geometry which includes a number of pin rods where the same situation occurs as in a one-dimensional cell, we, however, have no means than to apply the trapezoidal rule. We know that the finer interval of $\Delta\rho$ and $\Delta\varphi$ gives the more accurate results.

Implementation of this integration scheme requires the development of a tracing routine to calculate the intersections traversed by the line of integration. To maximize the computing efficiency, specialized routines are prepared for a variety of geometries which have been shown in Sect.2.4.

The calculation of collision probabilities is performed in two steps. First, the tracing routine is used to get the geometrical information called “trace table” by each line and accumulate on a large scale storage, say, disc. In the second step, these data, together with the cross sections, are used to perform the integration of collision probabilities. The second step is repeated for every energy group.

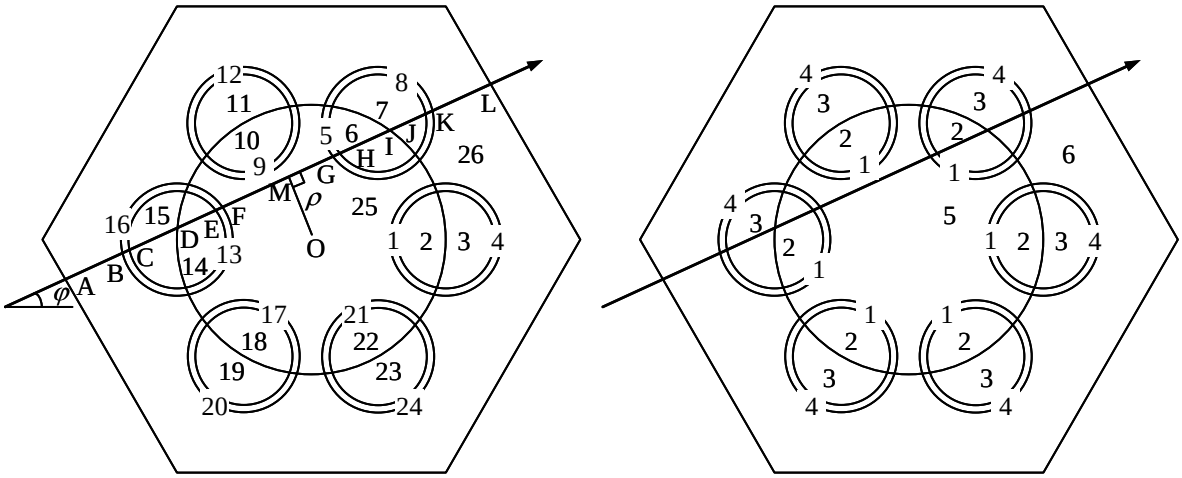
(1) How to Compose Trace Table

We shall describe how to compose the "trace table" using a sample geometry which is a hexagonal cell including six fuel rods equally spaced on a circular ring. Shown in Fig.7.1-6a are the purely geometrical region (S-Region) numbers. And the corresponding physical region (T-Region) numbers are indicated in Fig.7.1-6b. The latters are treated as the spatial variables after considering any symmetric condition. The rods consist of two concentric layers and they, together with the coolant, are divided further by the circle through the centers of the rods into inner and outer regions. Hence a

pin rod are divided into four regions. Since each rod is discriminated in the primary stage, the number of regions for rods amounts to 24. The inner and outer coolant regions are assigned by the succeeding numbers; 25 and 26.

A line (neutron path) defined by a pair of (ρ,φ) is drawn across the cell where ρ is the signed distance OM from the center of the cell O to the line, and φ is the angle made by this line and the horizontal line. The line intersects with the region boundaries at A,B,C,.....L. The point M (OM $\perp$ AL) is the origin of the measure on the line AL.

The preliminary trace table consists of an array `T` of which element is the signed distance from the point M to each intersecting point, an integer array `IR` for the region number of the right hand side of the point, and another array `IL` for the region number of the left hand side of the point.



a. S-Region map.　　b. T-Region map.

Fig.7.1-6　A hexagonal cell with six pin rods on a circle crossed by a line defined by a pair of parameters (ρ and φ)

The computing process is organized to find, first, the intersections A and L on the hexagonal boundary, then D and I on the circle through the rods centers. At this step, the preliminary trace table is made up as shown in Table 7.1-1.

Table 7.1-1　Preliminary trace table after scanning annular regions

Position	1	2	3	4
`T`	l_{AM}	l_{DM}	l_{MI}	l_{ML}
`IR`	26	25	26	-
`IL`	-	26	25	26

The next step is to scan whether the line intersects or not with any rod. This scanning is done, first, on the outermost radius of a rod. If judged to intersect, the information for the two crossing points with the circle is inserted into the table by a routine ”INSERT” which finds the positions in the table for the new two points rearranges the arrays `T`, `IR` and `IL` so that the elements may be in the geometrical order.

After the insertion, then, the scanning on the inner radius of the same pin rod is continued until the innermost radius if judged to intersect, otherwise the scanning is transferred to the next pin rod. After scanning all pin rods, the preliminary trace table is organized for the neutron line illustrated in Fig.8.1-6a as follows:

Table 7.1-2 Preliminary trace table after scanning all pin rods

k	1	2	3	4	5	6	7	8	9	10	11	12
T	l_{AM}	l_{BM}	l_{CM}	l_{DM}	l_{EM}	l_{FM}	l_{MG}	l_{MH}	l_{MI}	l_{MJ}	l_{MK}	l_{ML}
IR	26	16	15	14	13	25	5	6	7	8	26	-
IL	-	26	16	15	14	13	25	5	6	7	8	26

The final table is further rearranged as;

- Compose a new array `II` which keeps the T-Region numbers reduced from the array `IR` which keeps S-Region numbers using the correspondence specified in the input. Because of the 60° rotational symmetry, the common T-Region numbers are assigned to each pin rod region.
- Replace the element of `T` for the distance between the intersecting point and the point M by the distance between the two adjacent intersecting points.

Table 7.1-3 Final trace table at return step of geometry routine

k	1	2	3	4	5	6	7	8	9	10	11
T	l_{AB}	l_{BC}	l_{CD}	l_{DE}	l_{EF}	l_{FG}	l_{GH}	l_{HI}	l_{IJ}	l_{JK}	l_{KL}
II	6	4	3	2	1	5	1	2	3	4	6

The information obtained by the geometry routine is the common length of arrays, `L0`, the arrays `T` and `II` and the modified ρ value; ρ’ measured from the center of the adjacent cell which will be traced next if the perfect reflective boundary (mirror) condition is selected.

For the case of the mirror condition, the root routine calls repeatedly the same geometry routine with the adjusted arguments (ρ and φ) until the specified number of cells are traced, and concatenates

the arrays T and II, respectively.

Finally, a record per line keeps the following information:

W, L0, LLL, (T(*k*), *k*=1,2,,...,LLL), (II(k),*k*=1,2,...,LLL)

where W is the weight of a line given by

$$\mathtt{W} = 1 \qquad \text{for slab} \tag{7.1-73a}$$

$$\mathtt{W} = \omega_g (r_i - r_{i-1}) \quad \text{for} \quad r_{i-1} < \rho < r_i \qquad \text{for cylinder} \tag{7.1-73b}$$

$$\mathtt{W} = \rho \times \omega_g (r_i - r_{i-1}) \quad \text{for} \quad r_{i-1} < \rho < r_i \qquad \text{for sphere} \tag{7.1-73c}$$

$$\mathtt{W} = \Delta\rho \times \Delta\varphi = \text{constant} \qquad \text{for two-dimensional cylinder} \tag{7.1-73d}$$

where ω_g is the weight for the Gaussian quadrature at the point r_g in the range between r_{i-1} and r_i, and

- L0 : number of intersects of the source cell,
- LLL : total number of intersects on a line (Unless the mirror or periodic boundary condition is taken, LLL = L0),
- T(*k*) : distance between intersects which produces the optical thickness λ_k by multiplying the macroscopic cross-section of the region II(*k*),
- I(*k*) : region numbers of *k*-th intersect.

The total number of lines LCOUNT (records) required to achieve the integration varies widely depending on the complexity of the geometry, for example, LCOUNT= 2 for slab, LCOUNT= several tens for one-dimensional cylinder and sphere, and LCOUNT= a few thousands for the most complicated two-dimensional case.

After storing the trace tables for all lines, a numerical integration of region volumes and an array of integrated to exact volume ratios is printed as an indicator of the adequacy of the integration mesh. The numerical integration is performed by

$$\mathtt{V}(\mathtt{II}(k)) = \mathtt{V}(\mathtt{II}(k)) + \mathtt{W} \times \mathtt{T}(k) \quad \text{for } k=1,2,...,\mathtt{L0}$$

and accumulated by line. (7.1-74)

The resultant array V gives the numerically integrated region volumes.

(2) Process for Numerical Integration

Being given the cross sections of an energy group, the integration of collision probabilities is performed line by line. Actually, the symmetric element Δ_{ij} ($=V_i P_{ij} / \Sigma_j$) and Δ_{is} ($=V_i P_{is}$) are integrated instead of P_{ij} and P_{is}, respectively.

We shall show the computer process repeated by each line in the computational flow diagram

shown in Fig.7.1-7.

Information contained in a record;

W, L0, LLL, (T(k), k=1,2,...,LLL), (II(k), k=1,2,...,LLL)

The optical length λ_k is calculated by

λ_k = T(k) × {Cross section of II(k)} for k=1,2,..,LLL

Loop of source region, repeated for k=1,2,...,L0

i = II(k) ; source region number

$\lambda_i = \lambda_k$; optical thickness of source region

Set $\lambda_{ij} = 0$; optical distance between source region and collision region

Contribution to the diagonal element

$$\Delta_{ii}(\rho,\varphi) = \{F(0)\times\lambda_i - F(0) + F(\lambda_i)\} \ / \ \Sigma_i\Sigma_i$$

$$\Delta_{ii} = \int \mathrm{W}\times\Delta_{ii}(\rho,\varphi)d\rho d\varphi$$

Loop of collision region repeated for k'=k+1,...,LLL

j = II(k') ; collision region number

Set $\lambda_j \Leftarrow \lambda_{ij}$; optical thickness of collision region

Contribution to the off-diagonal element

$$\Delta_{ij}(\rho,\varphi) = \{F(\lambda_{ij}) - F(\lambda_{ij}+\lambda_i) - F(\lambda_{ij}+\lambda_j) + F(\lambda_{ij}+\lambda_i+\lambda_j)\} \ / \ \Sigma_i\Sigma_j$$

$$\Delta_{ij} = \int W\times\Delta_{ij}(\rho,\varphi)d\rho d\varphi$$

Prepare optical distance for the next k'

Set $\lambda_{ij} \Leftarrow \lambda_{ij} + \lambda_j$

End loop for collision region k'

unless the mirror condition (LLL > L0), then

Contribution to the escape element

$$\Delta_{is}(\rho,\varphi) = \{F(\lambda_{ij}) - F(\lambda_{ij}+\lambda_i)\}/\Sigma_i$$

$$\Delta_{is} = \int \mathrm{W}\times\Delta_{is}(\rho,\varphi)d\rho d\varphi$$

End loop for source region k

Fig.7.1-7 Computational flow-diagram for numerical integration by “Ray-Trace” method

The function $F(\lambda)$ appearing in the integrands in Fig.7.1-7 is given by

$F(\lambda) = E_{i3}(\lambda)$ for slab (7.1-75a)

$F(\lambda) = \exp(-\lambda)$ for sphere (7.1-75b)

$F(\lambda) = K_{i3}(\lambda)$ for one- and two-dimensional cylinder (7.1-75c)

Note that among four terms appearing in the expression of $\Delta_{ij}(\rho,\varphi)$, the first two terms have been calculated as the last two terms of the previous *k*'. The calculation of $\Delta_{ij}(\rho,\varphi)$ in the geometrical order reduces the number of transcendental functions to be evaluated into half.

Care is taken when λ_i is so small compared with unity so that differential approximations are used, for example,

$$K_{i3}(\lambda_{ij}) - K_{i3}(\lambda_{ij} + \lambda_i) \cong \lambda_i \times K_{i2}(\lambda_{ij}) \tag{7.1-76}$$

On integrating Δ_{ij}, the symmetric relation, $\Delta_{ij}=\Delta_{ji}$ validates to eliminate the loop of the source region in the reverse direction or to reduce the range of angular integration into half. The simple process to replace the off-diagonal element Δ_{ij} by $(\Delta_{ij} +\Delta_{ji})/2$ covers the above saving.

A normalization so that the sum of P_{ij} over *j* be unity is effective to reduce the error caused by coarse integration mesh, and also by truncated optical distance which is terminated by the fixed number of cells to be traced by neutron line for the perfect reflective boundary condition.

The numerical calculation of K_{in} functions has yet to be explained. Although some rational approximations are developed for the Bickley-Naylor functions[50], they would be very time consuming because they have to be used so frequently as 10^6~10^7 times. In the SRAC, a quadratic interpolation is performed numerically by using tables of **a**, **b**, **c**; the coefficients of three terms for the quadratic expression of the Bickley-Naylor function. These tables list **a**, **b** and **c** as a function of *x* and *n*, where

$$a_m = \frac{y_{m-1} - 2y_{m-1/2} + y_m}{2\Delta x^2} \tag{7.1-77a}$$

$$b_m = \frac{y_m - y_{m-1}}{\Delta x} - a_m(x_{m-1} + x_m) \tag{7.1-77b}$$

$$c_m = y_{m-1} - b_m x_{m-1} - a_m x_{m-1}^2 \tag{7.1-77c}$$

$$y_m = K_{in}(x_m) \tag{7.1-78}$$

$$\Delta x = (x_m - x_{m-1}) = 0.01 \tag{7.1-79}$$

The range of the tabulation of $K_{in}(x)$ is $0 \le x < 11.00$ for n=1, 5. In the range x>11.0, $K_{in}(x)$ is set to be zero, while the practical usage (by Fortran statements) may assume $K_{in}(x)$ vanishes if x>6.0.

Thus the Bickley-Naylor function is computed by performing twice the multiplication and twice the summation after table-look-up:

$$K_{in}(x) = (a_m x + b_m)x + c_m \tag{7.1-80}$$

where $x_{m-1} \le x \le x_m$

The table-look-up and the interpolation are performed in the routine itself to avoid the additional process of calling any external subroutine.

7.2 Optional Processes for Microscopic Total and Macroscopic Transport Cross-sections

This section is concerned with the options for the specification of the input data IC15 and IC16 in Sect.2.2. As these are related with transport property, care should be taken in processing moderating material. Discussions will be made on the optional treatment for microscopic total cross-section and for macroscopic transport cross-sections used in isotropic transport calculation and in evaluating diffusion coefficient.

7.2.1 Microscopic Total Cross-section

There are two ways to define the effective microscopic total cross-section in the SRAC system. In either way, the total cross-sections depend on all the compositions concerned.

(1) Optional Process IC15 = 1

One way is based on the concept of the Bondarenko type[51] cross-section set, i.e.,

$$\sigma_{t,g} = \sigma_{t,g}^{\infty} \; f_{t,g}(\sigma_0), \tag{7.2-1}$$

where the subscript g stands for energy group number, and $f_{t,g}(\sigma_0)$ is the self-shielding factor for the total cross-section. The total cross-section thus defined is efficient to maintain the diffusion coefficient evaluated in hyper-fine group structure in the multi-group constants.

(2) Optional Process IC15 = 2

On another way, the total cross-section is defined as the summation of all partial reaction cross-sections, i.e.,

$$\sigma_{t,g} = \sum_z \sigma_{z,g}^{\infty} \; f_{z,g}(\sigma_0) \tag{7.2-2}$$

where $f_{z,g}(\sigma_0)$ is the self-shielding factor for reaction type z.

7.2.2 Macroscopic Transport Cross-section

We start with the P_1 equations in multigroup representation[52]. The P_1 multigroup equations can be written as

$$\nabla \boldsymbol{J}_g(\boldsymbol{r}) + \Sigma_{t,g}\Phi_g(\boldsymbol{r}) = \sum_{g'} \Sigma_{s0,g'\to g} \; \Phi_{g'}(\boldsymbol{r}) + Q_g(\boldsymbol{r}) \tag{7.2-3}$$

$$\nabla \Phi_g(\boldsymbol{r}) + 3\Sigma_{t,g}\boldsymbol{J}_g(\boldsymbol{r}) = 3\sum_{g'} \Sigma_{s1,g'\to g}\boldsymbol{J}_{g'}(\boldsymbol{r}) \tag{7.2-4}$$

If a group-dependent form of Fick's law is postulated, i.e.,

$$\boldsymbol{J}_g(r) = -D_g(\boldsymbol{r})\nabla\Phi_g(\boldsymbol{r}) \tag{7.2-5}$$

then from Eq.(7.2-4) the diffusion coefficient can be formally expressed by

$$D_g(\boldsymbol{r}) = \frac{1}{3\Sigma_{tr,g}(\boldsymbol{r})} \tag{7.2-6}$$

with

$$\Sigma_{tr,g}(\boldsymbol{r}) \equiv \Sigma_{t,g} - \sum_{g'} \Sigma_{s1,g'\to g} \boldsymbol{J}_{g'}(\boldsymbol{r}) / \boldsymbol{J}_g(\boldsymbol{r}) \tag{7.2-7}$$

If the group width is wider compared with the maximum energy degradation of neutron by elastic collision and the quantity $E\boldsymbol{J}(\boldsymbol{r}, E)$ can be assumed to be energy-independent in the width, we can show[52)]

$$\sum_{g'} \Sigma_{s1,g'\to g} J_{g'}(\boldsymbol{r}) / J_g(\boldsymbol{r}) \cong \sum_{g'} \Sigma_{s1,g\to g'} = (\overline{\mu})_g \Sigma_{s,g} \tag{7.2-8}$$

in this case, we have

$$\Sigma_{tr,g}(\boldsymbol{r}) = \Sigma_{t,g} - \sum_{g'} \Sigma_{s1,g\to g'} \tag{7.2-9}$$

Four methods are prepared to define the transport cross-section to be used as total cross-sections in the isotropic transport calculation or diffusion calculation.

(1) Optional Process IC16 = 0

The first one treats simply the anisotropic scattering effect in the isotropic transport calculation by the extended transport approximation[23)]. Here, the macroscopic transport cross-section is defined by

$$\Sigma_{tr,g} = \Sigma_{t,g} - \sum_{g'} \Sigma_{s1,g\to g'} \tag{7.2-10}$$

It should be noted that the total cross-section, instead of the transport cross-section, is used to calculate the collision probability in the second resonance range, where the ultra-fine spectrum is calculated by assuming isotropic neutron scattering.

(2) Optional Process IC16 = 1 or 2

The second and third methods are based on the P_1 and B_1 approximation, respectively, for fast neutron spectrum calculation in homogeneous media[24)]. By choice of the option IC16= 1 or 2, the system under study is, first, homogenized by simple smearing of the atomic number densities in the cell, if IC2>0 is specified, and the P_1 and B_1 equations are solved by assuming an appropriate buckling.

Then, using the homogeneous spectrum obtained and assuming the flat flux, the effective cross-section of each material is calculated by

$$\Sigma_{tr,g,M} = \gamma_g \Sigma_{t,g,M} - \sum_{g'} \Sigma_{s1,g'\to g,M} \overline{\Phi}_{1,g'} / \overline{\Phi}_{1,g} \tag{7.2-11}$$

where

$$\gamma_g = 1 \qquad \text{for P1 approximation} \tag{7.2-12a}$$

$$\gamma_g = \alpha_g \tan^{-1}\alpha_g / 3\left\{1 - \left(\tan^{-1}\alpha_g\right)/\alpha_g\right\} \qquad \text{for B1 approx. with } \alpha^2{}_g = B^2/\Sigma^2_{t,g}, \text{ if } B^2>0 \tag{7.2-12b}$$

$$\gamma_g = \alpha_g \tanh^{-1}\alpha_g / 3\left\{1 - \left(\tanh^{-1}\alpha_g\right)/\alpha_g\right\} \qquad \text{for B1 approx. with with } \alpha^2{}_g = -B^2/\Sigma^2_{t,g}, \text{ if } B^2<0 \tag{7.2-12c}$$

Here, $\overline{\Phi}_{1,g}$ is the P_1 component of the angular flux, and B^2 is the geometrical buckling entered in Block-4 of Sect.2.2. This approach is recommended for the calculation of the lattice cell or homogeneous medium including hydrogenous material.

For an isolated material not used in the cell calculation or a new material used with an ‘old’ material which has already transport cross-sections, the above equation is solved in a system composed purely by the material.

(3) Optional Process IC16 = 3

The last method is based on the S_N transport calculation used for cell or core calculation. Here, the transport cross-section is defined, following to Eq.(7.2-7), by

$$\Sigma_{tr,g}(\boldsymbol{r}) = \Sigma_{t,g} - \sum_{g'} \Sigma_{s1,g'\to g} \Phi_{1,g'}(\boldsymbol{r}) / \Phi_{1,g}(\boldsymbol{r}) \tag{7.2-13}$$

This quantity is averaged over each volume or region in the system under consideration to give the representative value.

7.3 Optional Processes for Resonance Absorption

Concerning thermal and intermediate reactor analysis, a more accurate treatment, compared with fast reactor, is needed for the calculations of the effective resonance cross-sections in the lower energy regions. While the upper energy boundary of the energy range requiring the special attention was fixed to 130.07 eV, the latest SRAC version permits the extension to 961.07 eV. In this resonance energy range (called Resonance II range), three optional methods are available. The first one is based on a table-look-up method of resonance shielding factors, assuming the NRA (narrow resonance approximation) to the slowing down due to moderators, while the second IRA (intermediate resonance approximation) is assumed for the slowing down in the second one. In the third method, the effective cross-sections are exactly calculated by solving neutron slowing-down equation in heterogeneous system. These methods can be optionally chosen by the user.

On the first step of these calculations, the whole energy range is dealt with the table-look-up method assuming the NRA for moderator slowing-down. On the next step, the effective cross-sections in the second resonance energy range are replaced by the more accurate ones based on the IRA or the direct numerical method. Hence, in the higher energy range above Resonance II range, available is only the first method.

In the followings, descriptions will be given to the methods, which are incorporated in the SRAC system for calculating the effective resonance cross-sections.

7.3.1 Table-look-up Method of *f*-tables Based on NR Approximation in Homogeneous Systems

At first, consider an infinite homogeneous mixture consisting of one kind of resonance nuclide and of non-absorbing moderator. When the NRA is applied for the slowing down due to the moderator nuclide, the slowing down equation can be written as

$$\left\{ \sigma_t(u) + \sigma_b \right\} \varphi(u) = K(\sigma_s \varphi) + \sigma_b \tag{7.3.1-1}$$

with

$$\sigma_t(u) = \sigma_a(u) + \sigma_s(u) = \sigma_r(u) + \sigma_p \tag{7.3.1-2}$$

where $\varphi(u)$ is flux per unit lethargy, K, the slowing down operator, $\sigma_a(u)$, $\sigma_s(u)$, microscopic absorption and scattering cross-sections of the resonance absorber, respectively; $\sigma_r(u)$, and σ_p, the resonance part of total cross-section $\sigma_t(u)$ and the potential scattering cross-section, respectively, and σ_b is the scattering cross-section of the moderator.

Equation (7.3.1-1) is just the basic one that is used in the construction of the SRAC library for heavy resonance nuclides. That is, Eq.(7.3.1-1) with the Doppler broadened cross-sections by temperature T is rigorously solved with hyper-fine meshes for a given σ_b by the TIMS-1 code[17]. The calculated effective cross-sections are arranged by the infinite dilute cross-sections and the self-shielding factors $f(\sigma_b, T)$ tabulated by two parameters σ_b and T. Let us describe the way to use the shielding factors in practical situations.

For a special case where the NRA is applicable to the slowing down of absorber, the first-order solution can be written in the conventional form

$$\varphi(u) \cong \frac{\sigma_p + \sigma_b}{\sigma_t(u) + \sigma_b} \tag{7.3.1-3}$$

This first-order solution is usually adopted to construct a cross-section set of the Bondarenko type[51] with the resonance shielding factors for use in fast reactor analysis. For the higher energy region, say E > 130 eV, the NRA is considered to be a reasonable approximation for heavy nuclides. That is, the flux of Eq.(7.3.1-3) does not so much deviate from the exact one of Eq.(7.3.1-1) in the meaning of the weighting function for cross-section averaging. On the other hand, for the light and intermediate mass nuclides with resonance structure, the SRAC library has been generated assuming the spectrum of Eq.(7.3.1-3). In fact, no simple and convenient spectrum has been proposed to treat these nuclides. Since the resonance structure of light and intermediate mass nuclide is of minor importance in thermal and intermediate reactors, the present treatment will, in practice, be sufficient. Hence, we can think of Eq.(7.3.1-3) as representing a standard form of weighting spectrum for the higher energy regions.

For a homogeneous system including many moderator nuclides, the slowing down equation can be written as

$$\{\sigma_t(u) + \sigma_m\}\varphi(u) = K(\sigma_s\varphi) + \frac{1}{n_f}\sum_j n_j\sigma_j K_j(\varphi) \tag{7.3.1-4}$$

where $$\sigma_m = \frac{1}{n_f}\sum_j n_j\sigma_j \tag{7.3.1-5}$$

and K_j is the slowing down kernel for moderator j; n_f and n_j are the atomic number density of absorber and moderator nuclides, respectively.

When the NRA is applicable to the slowing down of moderators (referred to as NRA moderator), we have

$$\{\sigma_t(u) + \sigma_m\}\varphi(u) = K(\sigma_s\varphi) + \sigma_m \tag{7.3.1-6}$$

Consequently, a homogeneous system with the NRA moderators has the same effective cross-section as the homogeneous system described by Eq.(7.3.1-1). That is, the effective cross-sections can be calculated by calculating σ_m as to be used for the table-look-up of the resonance shielding tables. Here, it should be noted that the slowing down of absorber is still accurately estimated in the present treatment.

7.3.2 Table-look-up Method of *f*-tables Based on IR Approximation

We start with the IRA of resonance absorption in homogeneous systems, to give an insight into the relationship with the table-look-up method.

From the two extreme cases representing the limits of NR and wide resonance (WR) for the slowing down kernel, the first-order solution for $\varphi(u)$ of Eq.(7.3.1-1) can be written as[53), 54)]

$$\varphi(u) \cong \frac{\lambda\sigma_p + \sigma_b}{\sigma_a(u) + \lambda\sigma_s(u) + \sigma_b} \tag{7.3.2-1}$$

where λ is the IRA parameter for the absorber. The value of λ can be determined by solving a transcendental equation for λ [53, 54)].

For a homogeneous system including many moderator nuclides described by Eq.(7.3.1-4), the corresponding first-order solution can be given by

$$\varphi(u) \cong \frac{\lambda\sigma_p + \sigma'_b}{\sigma_a(u) + \lambda\sigma_s(u) + \sigma'_b} \tag{7.3.2-2}$$

with $$\sigma'_b = \frac{1}{n_f}\sum_j \lambda_j (n_j\sigma_j) \tag{7.3.2-3}$$

where λ_j is the IR parameter for moderator j and can be again determined by solving a coupled set of transcendental equations[54)].

Here, it should be noted that both the fluxes obtained from a numerical integration of Eq.(7.3.1-1) and given by Eq.(7.3.2-1) or (7.3.2-2) are the weighting functions for cross-section averaging. Hence, they can be assumed to give the same value for the effective cross-section in the extent of the accuracy of the IRA. Consequently, a homogeneous system with σ_b' has the same effective cross-section as the homogeneous system with the same σ_b of Eq.(7.3.1-1). That is, the effective cross-sections can be calculated by determining the IR parameters and σ_b' as to be used for the table-look-up of the resonance shielding tables. The case of letting all the λ_js equal to unity corresponds just to the NRA applied to the slowing down of moderators σ_b' = σ_m, as discussed in the previous subsection.

The IRA method described above can be applied only to a zero temperature system. For nonzero temperature, the IR parameter λ for absorber depends on temperature when the interference between potential and resonance scattering is taken into consideration[55)]. A simple way to take account of this dependence is to multiply the interference scattering term by a factor with temperature dependence[55)].

Next consider the IR treatment of resonance absorption in heterogeneous systems. Assuming a flat flux in each spatial region, the slowing down equation in the two-region system, consisting of an absorbing lump (f) and a non-absorbing moderator (m), can be written as

$$\sigma_f\varphi_f = p_{ff}\left\{\sigma_{am}K_{am}(\varphi_f) + K_f(\sigma_s\varphi_f)\right\} + (1-p_{ff})\sigma_f\sum_k\left\{R_k K_k(\varphi_m)\right\} \tag{7.3.2-4}$$

$$\sigma_f \varphi_f + \sigma_m \varphi_m = \sigma_{am} K_{am}(\varphi_f) + K_f(\sigma_s \varphi_f) + \sigma_m \sum_k \{R_k K_k(\varphi_m)\} \tag{7.3.2-5}$$

where

φ_f, φ_m = flux per unit lethargy in the lump and moderator region, respectively,

$\sigma_f(u) = \sigma_a(u) + \sigma_s(u) + \sigma_{am}$ = microscopic total cross-section of the lump,

$\sigma_{am} = \Sigma_{am} / n_f$ = scattering cross-section of admixed moderator per absorber atom,

$\sigma_m = \Sigma_m V_m / (n_f V_f)$, $R_k = \Sigma_k / \Sigma_m$, $\Sigma_m = \sum_k \Sigma_k$,

v_f, v_m = volumes of the lump and the moderator regions, respectively,

n_f = atomic number density of the resonance absorber in the lump,

K = slowing down operator,

p_{ff} = collision probability in the fuel lump.

The other notation is conventional.

We make use of the simple interpolation formula for the collision probability as proposed by Wigner:

$$p_{ff} = \frac{X}{X + g(C)(1-C)} = \frac{\sigma_f}{\sigma_f + s} \tag{7.3.2-6}$$

with $$X = l_f n_f \sigma_f = l_f \Sigma_f \tag{7.3.2-7}$$

$$s = g(C)(1-C)/(l_f n_f) \quad \text{and} \quad g(C) = \frac{a}{1 + (a-1)C} \tag{7.3.2-8}$$

where l_f : the lump mean chord length, C: the Dancoff correction factor and a is a purely geometrical quantity.

Generalized collision probability theory shows

$$p_{ff} \cong 1 - \frac{1-C}{X} \quad \text{for } X \to \infty \tag{7.3.2-9}$$

where the Dancoff correction factor C is zero for isolated lumps. Being based on Eq.(7.3.2-9), the Dancoff factor C is calculated by using the value of p_{ff} for a sufficiently large value of Σ_f as Σ_f = 300 cm^{-1}

$$1 - C = \{1 - p_{ff}(\Sigma_f)\} X \,|_{\Sigma_f \to \infty} \tag{7.3.2-10}$$

A rational interpolation of p_{ff} leads to $g(C)$ = 1 in Eq.(7.3.2-6) when use is made only of the behavior of p_{ff} at $\Sigma_f \to \infty$ given by Eq.(7.3.2-9). Since the bulk of resonance absorption occurs at finite values of Σ_f, we need some corrections for the rational approximation. It is this quantity a that

has been introduced for the corrections[56,57,58]. Since the quantity, *a*, usually referred to as the Bell or Levine factor, somewhat fluctuates among resonance levels, there might be some minor problems with the choice. The exact choice of this quantity is not thought to be important, considering from the results of many studies done in this field[58]. The values adopted in the SRAC system for the geometric quantities are shown in the following table.

Table 7.3.2-1 Levine or Bell Factors

Geometry	l_f	*a*	Remarks
Sphere of radius *r*	4*r*/3	1.4	cf. 27), 59)
Slab of thickness *r*	2*r*	1.2	cf. 27), 19)
Infinite cylinder of radius *r*	2*r*	1.2	cf. 56), 57)
Infinite hollow cylinder of inner radius *a* and outer radius *b*, $\sin\theta=a/b$	$2r\cos^2\theta$	1.2	cf. 59), 60)

The Dancoff correction factor and associated quantities will be in more general form discussed for multi-region problems in the next subsection.

Substituting Eq.(7.3.2-6) into Eq.(7.3.2-4) and subtracting Eq.(7.3.2-5) from the resulting equation, we obtain the following set of equations for neutron balance:

$$(\sigma_f + s)\varphi_f = \sigma_{am} K_{am}(\varphi_f) + K_f(\sigma_s \varphi_f) + s\sum_k \{R_k K_k(\varphi_m)\} \tag{7.3.2-11}$$

$$s\varphi_f = \sigma_m \varphi_m + (s - \sigma_m)\sum_k \{R_k K_k(\varphi_m)\} \tag{7.3.2-12}$$

Then, from the two extreme cases representing the limits of NR and WR, respectively, for the slowing down kernels, the first-order solution for φ_f and φ_m can be written as[21]

$$\varphi_f^{(1)}(u) = \frac{\lambda\sigma_p + \kappa\sigma_{am} + \mu^* s}{\sigma_a + \lambda\sigma_s + \kappa\sigma_{am} + \mu^* s} \tag{7.3.2-13}$$

$$\varphi_m^{(1)}(u) = 1 - s\left\{1 - \varphi_f^{(1)}(u)\right\} \Big/ \{\mu\sigma_m + (1-\mu)s\} \tag{7.3.2-14}$$

with

$$\mu^* = \mu\sigma_m / \{\mu\sigma_m + (1-\mu)s\} \quad \text{and} \quad \mu = \sum_k R_k \mu_k \tag{7.3.2-15}$$

where μ_k is the IR parameter for the outside moderator *k*. Here, a set of the IR parameters can be determined by the same procedure as those in a homogeneous system[21].

Equation(7.3.2-13) can be written in the standard form of Eq.(7.3.2-1):

$$\varphi_f^{(1)}(u) = \frac{\lambda\sigma_p + \sigma_b}{\sigma_a + \lambda\sigma_s + \sigma_b} \tag{7.3.2-16}$$

where

$$\sigma_b = \kappa\sigma_{am} + \mu^* s = \frac{\kappa\Sigma_{am}}{n_f} + \frac{\mu^* g(C)(1-C)}{n_f l_f} \tag{7.3.2-17}$$

Particularly for the NRA (κ=1, μ^*=1), the above equation can generally be written as

$$\sigma_b = \sigma_{am} + s = \frac{1}{n_f}\sum_{j\neq f} n_j\sigma_j + \frac{g(C)(1-C)}{n_f l_f} \tag{7.3.2-18}$$

The simple result of Eqs.(7.3.2-17) and (7.3.2-18) again reveals the following equivalence relation with practical usefulness: A heterogeneous system with σ_b has the same effective resonance cross-section as a homogeneous system of Eq.(7.3.1-1) with the same σ_b. In other words, the effective cross-sections in a heterogeneous system can be estimated by using a cross-section set of the Bondarenko type[51] which is calculated based on Eq.(7.3.1-1).

Several groups of the multigroup structure around 100 eV include more than one resonance levels of ^{238}U. Since the background cross-section σ_b somewhat fluctuates among the resonance levels, the arithmetic average value of σ_b's in each group is in practice taken as the background cross-section for the table-look-up. In the SRAC system, the IR method is applied only to ^{238}U, ^{232}Th, and ^{240}Pu.

7.3.3 Generalized Dancoff Correction Factor

The effective resonance cross-sections in heterogeneous systems have been calculated by combined use of an equivalence theorem[61] and a cross-section set of the Bondarenko type[51]. The equivalence theorem between homogeneous and heterogeneous systems is usually established through a Dancoff correction factor. This factor has been derived under the assumption that the system under study consists of an infinite array of two-region cells. Meneghetti[62] derived a generalized Dancoff correction factor for a more general situation of infinite array of multi-region plate cell. In a complex situation as encountered in the lattice of the PROTEUS-LWHCR (Light Water High Converter Reactor) cores[63] where MOX pin and depleted U pin are alternatively placed in a hexagonal array, however, it is generally difficult to see how one can construct a unit cell for which the Dancoff correction factor can be calculated. A generalized Dancoff correction factor was derived for infinite array of multi-region cells including several absorber lumps with different absorber densities[19]. The equivalence theorem based on this Dancoff correction factor is incorporated in the SRAC system.

The neutron slowing-down equation in a cell may be written by using the collision probabilities

$$\varphi_i(u) = \sum_j P_{ij}(u) W_j(u) X_{0j} / X_j(u) \quad , \tag{7.3.3-1}$$

$$W_j(u) = S_j(u) / \Sigma_{0j} \quad , \tag{7.3.3-2}$$

$$X_{0j}(u) = \bar{l}_j \Sigma_{0j} \ , \qquad X_j = \bar{l}_j \Sigma_j(u) \quad , \tag{7.3.3-3}$$

where the subscript j denotes a spatial region j, $S_j(u)$ the slowing-down source, $\bar{l}_j$, the mean chord length, Σ_{0j}, the non-resonance part of $\Sigma_j(u)$ and the other notation is conventional.

Now, let us consider the limit at which the resonance cross-section of one resonant isotope, say σ_t, tends to be infinite. This black limit corresponds to a physical situation encountered near a resonance energy. Then, all the macroscopic cross-sections of the region with the resonance isotope under consideration will also tend to be infinite. We denote these regions by the symbol R.

General arguments on asymptotic behaviors of the collision probability, P_{ij}, at the black limit[27), 64), 65)] show

$$P_{ij}(\sigma_t) \equiv P_{ij}(u) \to \delta_{ij} - \gamma_{ij} / X_i \qquad (i \in R) \quad \text{for} \quad X_i \to \infty \tag{7.3.3-4}$$

with $$\gamma_{ij} \equiv \lim_{\sigma_t \to \infty} \{\delta_{ij} - P_{ij}(\sigma_t)\} X_i \quad . \tag{7.3.3-5}$$

From the conservation law

$$\sum_j P_{ij} \equiv 1 \tag{7.3.3-6}$$

we have

$$\sum_j \gamma_{ij} \equiv 0 \quad \text{or} \quad \gamma_{ii} = -\sum_{j \neq i} \gamma_{ij} \quad . \tag{7.3.3-7}$$

Therefore, we have for the flux $\varphi_i(u)\ (i \in R)$

$$\varphi_i(u) \to \left(W_i^{\infty} X_{0i} - \sum_{j \notin R} W_j^{\infty} X_{0j} \gamma_{ij} / X_j \right) \Big/ X_i + O\left(X_i^{-2}\right) \quad \text{for} \quad X_i \to \infty \tag{7.3.3-8}$$

$$W_j^{\infty} \equiv \lim_{\sigma_t \to \infty} W_j \quad . \tag{7.3.3-9}$$

Here, since we try to treat the higher energy region, say $E \geq$ several hundred eV, the NRA is a reasonable approximation, i.e.,

$$W_j(u) = const. \equiv 1 \quad . \tag{7.3.3-10}$$

Moreover, we assume that accidental overlapping between different resonance sequences is negligible,

i.e.,

$$X_{0j} / X_j = 1 \quad (j \notin R) \quad . \tag{7.3.3-11}$$

Under these assumptions, Eq.(7.3.3-8) can be rewritten as

$$\varphi_i(u) \to \left(X_{0i} - \sum_{j \notin R} \gamma_{ij} \right) \Big/ X_i \quad \text{for} \quad X_i \to \infty \quad . \tag{7.3.3-12}$$

On the other hand, an equivalent theorem between homogeneous and heterogeneous systems means that the flux in the absorber lump should be expressed by the spectrum in homogeneous medium

$$\varphi_i(u) = \frac{X_{0i} + b_i}{X_i + b_i} \to (X_{0i} + b_i) / X_i \quad \text{for} \quad X_i \to \infty \quad . \tag{7.3.3-13}$$

where the flux is normalized to be unity at off-resonance energy.

For Eqs.(7.3.3-12) and (7.3.3-13) to be held, the following identity must be satisfied:

$$b_i = - \sum_{j \notin R} \gamma_{ij} \tag{7.3.3-14}$$

For a special case where the unit cell under study consists of fuel region (*f*) and moderator region (*m*), we can prove the conventional relation[61)]

$$b_i = - \gamma_{fm} = 1 - C \quad , \tag{7.3.3-15}$$

where C is the Dancoff correction factor and $-\gamma_{fm}$ corresponds to the first-flight blackness for neutrons leaving the fuel region[61)]. Figure 7.3.3-1 shows the expression of b_i for other simple geometries.

Consequently, from the above examples, Eq.(7.3.3-14) is considered to be a generalization of the previous works introduced in the previous section. Equation (7.3.3-14) shows that the Dancoff correction factor for complex geometry can be obtained by calculating the generalized blackness γ_{fm}. Here, the blackness γ_{fm} is calculated by using the collision probability package in the SRAC system, that is, by using the value of P_{ij} for a sufficiently large value of Σ_j $(j \in R)$, as Σ_j=300 cm^{-1}, based on Eq.(7.3.3-5).

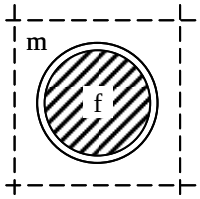
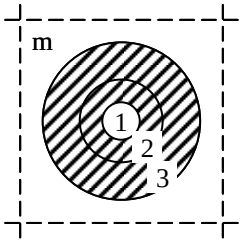
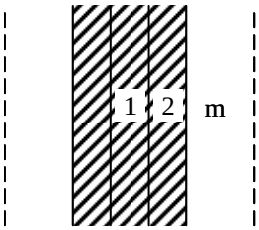
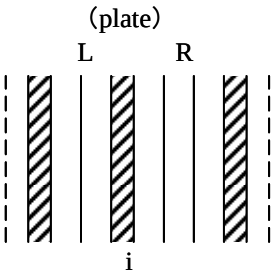
Geometry	b_i
	$b_f = -(\gamma_{fc} + \gamma_{fm}) > 0$
	$b_i = \begin{cases} 0 & i=1 \\ 0 & i=2 \\ \gamma_{33} = -\gamma_{3m} > 0 & i=3 \end{cases}$
	$b_i = \begin{cases} 0 & i=1 \\ \gamma_{22} = -\sum_m \gamma_{2m} > 0 & i=2 \end{cases}$
	$b_i = 1 - E_3(X_L) - E_3(X_R)$ $X \equiv \sum_m d_m \Sigma_m$ Meneghetti's two-sided formula

Fig. 7.3.3-1 Dancoff correction factors for simple geometries

The symbol (*m*) means moderator region and the shaded portions show the R-region: The quantities d_m stands for the width of moderator plate *m*.

The equation (7.3.3-13) can be rewritten in a standard form of weighting spectrum

$$\varphi_i(u) = \frac{\sigma_p + \sigma_{bi}}{\sigma_t(u) + \sigma_{bi}} \tag{7.3.3-16}$$

$$\sigma_{bi} = \frac{1}{n_i}\sum_{j\neq i} n_j \sigma_j + \frac{b_i}{n_i l_i} \quad , \tag{7.3.3-17}$$

where n_i and n_j are the atomic number densities of the absorber under consideration and of admixed moderators, respectively.

The standard spectrum of Eq.(7.3.3-16) was obtained again from the behavior of the collision probability at $\sigma_t \to \infty$. So we need some corrections for the present approach, as done in the previous section. For this purpose we at first define the generalized Dancoff correction factor of an absorber in the region *i* by

$$C_i = 1 - b_i \tag{7.3.3-18}$$

Then the two-region problem in the previous subsection suggests the replacement of (1 - C_i) by (1 - C_i)g(C_i) with

$$g(C_i) = \frac{a}{1 + (a-1)C_i} \quad . \tag{7.3.3-19}$$

Accordingly we can generally define the background cross-section, σ_{bi}, including the heterogeneity by

$$\sigma_{bi} = \frac{1}{n_i}\sum_{j\neq i} n_j \sigma_j + \frac{g(C_i)(1-C_i)}{n_i l_i} \quad . \tag{7.3.3-20}$$

Here, the value of the Bell factor, *a*, of Eq.(7.3.3-19) is assumed to take the respective value of Table 7.3.2-1 corresponding to the geometry under consideration.

We again obtain the equivalence relation: The effective cross-sections of absorber nuclides in each region can be calculated by using a cross-section set of the Bondarenko type.

In the resonance energy range I ($E \geq 130.07$ eV), the effective cross-sections are obtained by the table-look-up method of a Bondarenko type cross-section set, where the heterogeneity is treated by the established equivalence relation of Eq.(7.3.3-20) between heterogeneous and homogeneous mixtures. The cross-sections in the second region (130.07 eV $\geq E \geq$ 0.414 eV are generally calculated by the IRA or a direct numerical method using collision probability and hyper-fine group width (Δu = 0.00125), as described in the next subsection. Hence, the energy range concerning the present improvement is mainly the first resonance region.

As known through the present derivation, each resonant nuclide in one absorber lump may take a different value for the generalized Dancoff correction factor. One example of this type of problems

will be seen in the reference[65]. Moreover, there might be a problem whether or not we should treat a region with small amount of resonance absorbers as the R-Region; this problem would not be essential, since the effective cross-sections in such a region should be nearly infinite dilution cross-sections. Anyway, a complex heterogeneity can be treated consistently without introducing any simplification of geometry.

7.3.4 Direct Method for Calculating Neutron Flux Distribution (the Method in 'PEACO')

We assume that heterogeneous systems are built up of an infinite number of 'unit cells' and the neutron balance in a heterogeneous system can be described by using the first-flight collision probabilities. To reduce the numerical errors caused by the flat-flux assumption, each region of the system may be divided into sub-regions as many as necessary or possible. Then, assuming the isotropic elastic scattering, the neutron balance in a cell may be written by the neutron slowing down equation

$$V_i \Sigma_i(u)\Psi_i(u) = \sum_{j=1}^{J} P_{ji}(u) V_j \sum_{k=1}^{K} S_{jk}(u) \tag{7.3.4-1}$$

$$S_{jk}(u) = \frac{1}{1-\alpha_k} \int_{u-\varepsilon_k}^{u} \exp\{-(u-u')\} \Sigma_{s\,jk}(u')\Psi_j(u')du' \tag{7.3.4-2}$$

with

$$\alpha_k = \left(\frac{A_k - 1}{A_k + 1} \right)^2 \quad \text{and} \quad \varepsilon_k = -\ln \alpha_k \tag{7.3.4-3}$$

Here, the subscripts *i* and *j* stands for the sub-region number and the *k* corresponds to nuclear species. The quantity P_{ji} is the effective probability in a unit cell that a neutron scattered isotropically in region *j* into lethargy *u* will have its first collision in region *i* and other notation has the customary meanings. By letting $V_i \Psi_i(u) \exp(u) = \Psi_i(u)$, we have

$$\Sigma_i(u)\Psi_i(u) = \sum_j \sum_k P_{ji}(u) S^0{}_{jk}(u) \tag{7.3.4-4}$$

$$\text{with} \quad S^0{}_{jk}(u) = \frac{1}{1-\alpha_k} \int_{u-\varepsilon_k}^{u} F_{jk}(u')du' \tag{7.3.4-5}$$

$$F_{jk}(u) = \Sigma_{s\,jk}(u)\Psi_j(u) \tag{7.3.4-6}$$

Here, note that the equations (7.3.4-4) and (7.3.4-5) for $\Psi_i(u)$ is more simple than Eqs.(7.3.4-1) and (7.3.4-2).

For the computation of the neutron spectrum $\Psi_i(u)$ on discrete lethargy meshes, we use the RABBLE Method developed by Kier[22, 66]. Hence, the lethargy meshes used are assumed to be extremely narrow compared to the maximum lethargy gain per collision with the heaviest nuclides in the system under consideration. Furthermore, we assume that the resonance cross-sections are given at the mid-point of this fine group and the collision probabilities $P_{ji}(u)$ is constant over a fine group. Now define

$$\Psi_i^m = \int_{u_o}^{u_+} \Psi_i(u)du \tag{7.3.4-7}$$

$$F_{jk}^m = \int_{u_0}^{u_+} F_{jk}(u)du = \Sigma_{s\,jk}^m \Psi_j^m \tag{7.3.4-8}$$

where u_+ and u_0 are upper and lower lethargy bounds, respectively, corresponding to the fine group m. Then, the integration of Eq.(7.3.4-4) over the lethargy range from u_0 to u_+ gives

$$\Sigma_i^m \Psi_i^m = \sum_{j,k} P_{ji}^m Q_{jk}^m \tag{7.3.4-9}$$

where

$$Q_{jk}^m = \frac{1}{1-\alpha_k} \int_{u_0}^{u_+} du \int_{u-\varepsilon_k}^{u} F_{jk}(u')du' \tag{7.3.4-10}$$

$$\cong \frac{\Delta u_m}{1-\alpha_k} \int_{u-\varepsilon_k}^{u} F_{jk}(u')du'$$

$$= Q_{jk}^{m-1} + \frac{\Delta u_m}{1-\alpha_k} \left\{ F_{jk}^m - (F_{jk})^{m-L_k^m} \right\} \tag{7.3.4-11}$$

with $$\left(F_{jk}\right)^{m-L_k^m} = \int_{u_- -\varepsilon_k}^{u_0-\varepsilon_k} F_{jk}(u)du \tag{7.3.4-12}$$

Here, u_- is the lower bound of the (m-1)th fine group and L_k^m is an integral number of groups which corresponds of the maximum lethargy gain by elastic collision. Note that the self-scatter was neglected in deriving the above equations because the effect of the self-scatter was shown to be quite insignificant[67].

It is moreover assumed that the scattering rate given by Eq.(7.3.4-12) can be approximated by using the intermediate group scattering rate[66]. The accuracy of this approximation was also investigated and shown to be quite satisfactory when an adequate group structure is adopted for representing the fine and intermediate groups[67]. Assuming the asymptotic flux distribution below the lethargy range under consideration, the neutron flux distribution can be recursively calculated, until the entire energy range of interest is covered.

The lattice cell under study may consist of several materials and each may be subdivided into several spatial regions. The resonance-absorbing isotopes are contained in some materials (fuel-materials) and other materials are assumed to have constant cross-sections. Now, for such a system we select a resonance absorber, say ^{238}U and define the microscopic resonance cross-section per the absorber under consideration in the fuel materials by

$$\bar{\sigma}_I(E) = \frac{1}{N_I}\sum_k N_{Ik}\sigma_k(E) \qquad (N_I \neq 0) \tag{7.3.4-13}$$

where I corresponds to the fuel material, the summation on k is extended over all the resonance absorbers, $\sigma_k(E)$ is the microscopic total cross-section of the k-th absorber, and N_I and N_{Ik} are the atomic number densities of the absorber under consideration and of the k resonance absorber in the I-th material, respectively.

Some fuel materials may have the same relative densities N_{Ik} / N_I, hence the same value for $\bar{\sigma}_I(E)$. In such materials, the value of $\bar{\sigma}_I(E)$ can be considered as a common variable to express the macroscopic total cross-sections. There may be another possibility to find such an independent variable in other fuel materials. In the present treatment, it is assumed that the macroscopic total cross-sections can be expressed or be approximated by using at most two such independent variables.

Now, let us denote by Σ_{0J} the smallest macroscopic total cross-section made by the non-resonant isotopes in the fuel material J belonging to the independent variable $\bar{\sigma}_J(E)$. Let us introduce new variables defined by

$$X_J = (N_J\bar{\sigma}_J + \Sigma_{0J})\bar{l}_J \qquad (J = 1, \mathrm{JMAX}) \tag{7.3.4-14}$$

where JMAX is the number of the independent variables ($\mathrm{JMAX} \leq 2$) and $\bar{l}_J$ is a parameter with dimension of length introduced to define the non-dimensional variable X_J and assumes the averaged value of double widths of the regions which belong to the variable $\bar{\sigma}_J(E)$. Then, the collision probability, $P_{ji}(u)$ in Eqs.(7.3.4-1) or (7.3.4-5) can be considered to be a function of X_J (J=1, JMAX).

In the routine 'PEACO', two kinds of computational methods are adopted for the calculation of X_J (J=1, JMAX). In the first method which is used for the values of X_1, $X_2 \leq 9$, $P_{ji}(X_1, X_2)$ needed for the interpolation are calculated by calling the routine 'PIJ2'. The second one uses the asymptotic expansion of $P_{ji}(X_1, X_2)$ when either X_1 or $X_2 \geq 9$.

(1) One resonance-absorbing composition problem (JMAX=1)

It is easy to show[27), 65), 68)]

$$P_{ij}(X) \to \eta_{ij} + \gamma_{ij} / X \qquad \text{for} \quad X \to \infty \tag{7.3.4-15}$$

with $$\eta_{ij} \equiv P_{ij}(X = \infty) \tag{7.3.4-16}$$

and $$\gamma_{ij} \equiv \begin{cases} 0 & \text{if } i \notin R \\ \{P_{ij}(X) - \eta_{ij}\} X \mid_{X \to \infty} & \text{if } i \in R \end{cases} \tag{7.3.4-17}$$

where R stands for the resonance-absorbing material.

The above equation (7.3.4-15) is used for X>9 and the generalized Dancoff correction factor γ_{ij} given by Eq.(7.3.4-17) is calculated at X=9, while η_{ij} is obtained as the value of $P_{ij}(X)$ at X=104.

On the other hand, for the range of X<9, we introduce a new variable

$$Z \equiv \frac{X}{X+1} \qquad \text{or} \qquad X = \frac{Z}{1-Z} \quad . \tag{7.3.4-18}$$

The interpolation of the collision probability is made by using the values of $P_{ij}(X)$ calculated on ten points of the variable Z with the increment ΔZ=0.1 and the Lagrangian three points interpolation formula[69)]

$$f(Z_0 + \delta Z) = \frac{1}{2} u(u-1) f_{-1} + (1-u^2) f_0 + \frac{1}{2} u(u+1) f_1 \tag{7.3.4-19}$$

with $$u = \frac{\delta Z}{\Delta Z} \qquad \text{and} \qquad |u| \le 1, \tag{7.3.4-20}$$

where the quantity ΔZ is the mesh width of the variable Z at Z=Z_0 corresponding to the direction of the increment δZ.

The values of Z and X used for the interpolation are shown in the following table:

Table 7.3.4-1

No.	Z	X
1	0	0
2	0.1	0.111111
3	0.2	0.25
4	0.3	0.428571
5	0.4	0.666667
6	0.5	1.
7	0.6	1.5
8	0.7	2.333333
9	0.8	4.
10	0.9	9.
11	0.9999	10E+4

(2) Two resonance-absorbing composition problem (JMAX=2)

We can prove also for the two resonance-absorbing mixtures, R_1, R_2

$$P_{ij}(X_1, X_2) \approx \begin{cases} P_{ij}(\infty, X_2) - \gamma_{ij}^1(X_2)/X_1 & X_1 > 9, X_2 \le 9 \\ \quad (\gamma_{ij}^1(X_2) \equiv 0 \quad \text{if } i \notin R_1) & \\ P_{ij}(X_1, \infty) - \gamma_{ij}^2(X_1)/X_2 & X_1 \le 9, X_2 > 9 \\ \quad (\gamma_{ij}^2(X_1) \equiv 0 \quad \text{if } i \notin R^2) & \end{cases} \tag{7.3.4-21}$$

$$P_{ij}(X_1, X_2) \approx \begin{cases} P_{ij}(\infty, \infty) - \gamma_{ij}^{\infty}/X_1 & \text{if } i \in R_1 \text{ and } X_1, X_2 > 9 \\ P_{ij}(\infty, \infty) - \gamma_{ij}^{\infty}/X_2 & \text{if } i \in R_2 \text{ and } X_1, X_2 > 9 \\ P_{ij}(\infty, \infty) & \text{otherwise} \end{cases} \tag{7.3.4-22}$$

Here, P_{ij} and γ_{ij} in Eq.(7.3.4-21) is calculated by the exactly same way as the case of the interpolation of $P_{ij}(X)$ for $X<9$ in the one resonance-absorbing composition problem.

For the range of $X_1, X_2 \le 9$, we again introduce two variables

$$Z_I \equiv \frac{X_I}{X_I + 1} \qquad \text{or} \qquad X_I = \frac{Z_I}{1 - Z_I} \qquad (I = 1,2) \tag{7.3.4-23}$$

and $P_{ij}(X_1, X_2)$ is interpolated on the these variables by using one of the following formulae[69)]

$$\begin{aligned} f(Z_{10} + \delta Z_1,\ Z_{20} + \delta Z_2) = & \left\{1 - \frac{1}{2}(3 - u - \upsilon)(u + \upsilon)\right\} f_{00} \\ & + (2 - u - \upsilon)(u\, f_{10} + \upsilon\, f_{01}) + u\upsilon\, f_{11} \\ & + \frac{1}{2}u(u-1) f_{20} + \frac{1}{2}\upsilon(\upsilon - 1) f_{02} \end{aligned} \tag{7.3.4-24}$$

with $\quad u = \dfrac{\delta Z_1}{\Delta Z_1} \quad , \quad \upsilon = \dfrac{\delta Z_2}{\Delta Z_2} \quad , \quad |u| \le 1 \quad , \quad |\upsilon| \le 1 \quad ,$ (7.3.4-25)

$$\begin{aligned} f(Z_{10} + \delta Z_1, Z_{20} + \delta Z_2) = & \frac{1}{2}u(u-1) f_{-10} + \frac{1}{2}\upsilon(\upsilon - 1) f_{0-1} \\ & + (1 - u\upsilon - u^2 - \upsilon^2) f_{00} + \frac{1}{2}u(u - 2\upsilon - 1) f_{10} \\ & + \frac{1}{2}\upsilon(\upsilon - 2u + 1) f_{01} + u\upsilon\, f_{11} \quad , \end{aligned} \tag{7.3.4-26}$$

$$\begin{aligned} & f(Z_{10} + \delta Z_1, Z_{20} + \delta Z_2) \\ & \quad = (1-u)(1-\upsilon) f_{00} + u(1-\upsilon) f_{10} + \upsilon(1-u) f_{01} + u\upsilon\, f_{11} \, . \end{aligned} \tag{7.3.4-27}$$

The choice of Eqs.(7.3.4-24), (7.3.4-26) or (7.3.4-27) depends on the values of Z_1, Z_2 on which the $P_{ij}(X_1, X_2)$ is to be interpolated.

(3) Conservation and reciprocity of collision probabilities

The first-flight collision probability must satisfy the two important relations, that is, the conservation law

$$\sum_j P_{ij} = 1 \qquad \text{for all} \quad i \tag{7.3.4-28}$$

and the reciprocity relation[61)]

$$V_i \Sigma_i P_{ij} = V_j \Sigma_j P_{ji} \qquad \text{for all} \quad i, j. \tag{7.3.4-29}$$

In the routine 'PEACO', at first, the values of P_{ij} are calculated only for $i \leq j$ by Eqs.(7.3.4-15) and (7.3.4-27). Then, the collision probabilities satisfying Eqs.(7.3.4-28) and (7.3.4-29) are successively obtained by the following equations starting from i=1:

$$P_{ij}^{\ *} = \frac{1-\beta_1}{\beta_0} P_{ij} \quad , \quad P_{ji}^{\ *} = \frac{1-\beta_1}{\beta_0} P_{ji} \quad (j = i, J) \quad , \tag{7.3.4-30}$$

where $$\beta_0 = \sum_{j=1}^{J} P_{ij} \qquad \text{and} \qquad \beta_1 = \sum_{i=1}^{j-1} P_{ij}^{\ *} \quad , \tag{7.3.4-31}$$

with $$P_{ij} \;=\; V_j \Sigma_j P_{ji} / \left(V_i \Sigma_i\right) \qquad \text{for} \quad i < j \,. \tag{7.3.4-32}$$

The collision probabilities $P_{ij}^{\ *}$ given by Eq.(7.3.4-30) will be readily known to satisfy Eqs.(7.3.4-28) and (7.3.4-29).

Using the interpolation and the asymptotic expansion, combined with the methods mentioned above, we can guarantee the accuracy of 0.1% for the calculation of the collision probability, including the one resonance-absorbing mixture problem. Furthermore it should be emphasized that most of practical problems can be executed in a computing time of the same order as the convenient method based on the IRA.

7.3.5 Resonance Absorption in Doubly Heterogeneous System

The HTTR (High Temperature Engineering Test Reactor): an HTGR, constructed at JAEA, uses fuel in the form of small spherical coated particles. A coated particle consists of a fuel kernel of UO_2 with an ~600 μm diameter and several layers of pyrolytic carbon and SiC of ~150 μm thickness. Such coated particles, together with graphite diluent, are formed into hollow annular fuel compacts that are packed in a graphite sleeve, and then inserted into a graphite block (See Fig.7.3.5-1).

One of the physical problems associated with this type of fuel is a double heterogeneity through the self-shielding of the grain and also of the lattice configuration of fuel rods on the resonance absorption.

Here, the "Accretion" method by Leslie & Jonsson[70] to calculate collision probabilities in a cluster-type fuel element is applied to evaluate the resonance absorption in the doubly heterogeneous system in the fuel block of the HTTR. The details will be found in the reference[26] together with some typical numerical examples.

We assume that the fuel grains in a fuel compact are uniformly distributed so that each coated particle, together with graphite diluent, forms a two-region spherical cell (microscopic cell) containing only a fuel grain (region *f*) and the associated amount of graphite diluent (region *m*).

The neutron slowing-down equations can be written by using the collision probabilities under the assumption that the neutron flux is flat in each spatial region and the neutron scattering is isotropic and elastic:

$$V_j \Sigma_j(u)\varphi_j(u) = \sum_i P_{ij}(u) V_i S_i(u) \quad , \tag{7.3.5-1}$$

$$S_i(u) = \int_0^u \Sigma_i(u' \rightarrow u)\varphi_i(u')du' \quad , \tag{7.3.5-2}$$

where V_i, Σ_i, φ_i, $\Sigma_i(u' \rightarrow u)$, and S_i are the volume, the total cross-section, the neutron flux, the differential scattering cross-section, and the slowing down source of the *i*-th region, respectively. The quantity P_{ij} is the collision probability that a neutron emitted in the region *i* has the next collision in the region *j*, evaluated by assuming the flat flux in each region.

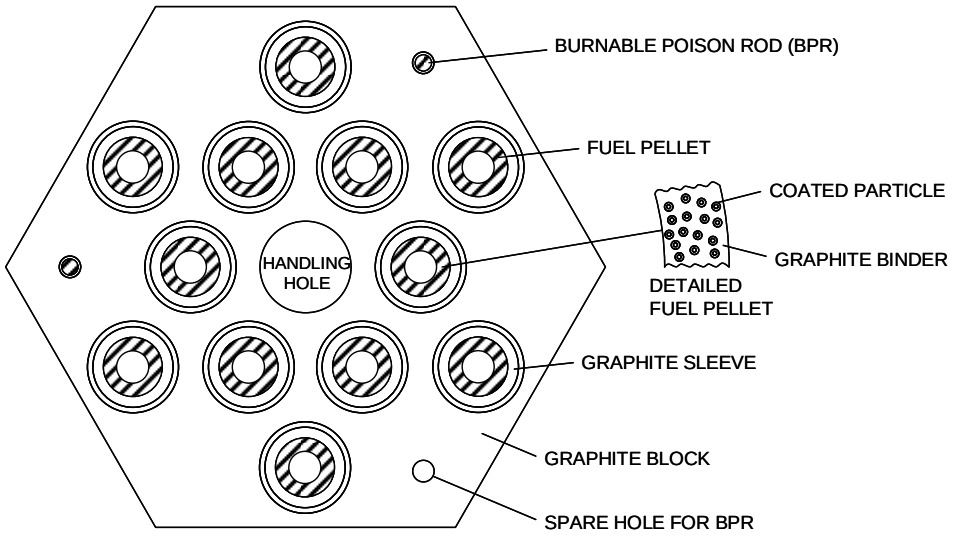


Fig.7.3.5-1 Horizontal cross-section of the standard fuel block of the VHTRC

VHTRC: Very High Temperature Reactor Critical Assembly, decommissioned

When we consider the doubly heterogeneous case as seen in the HTTR block, each region must be specified as l in I to denote the microscopic region l (= f or m) in the macroscopic region I. Hence, the collision probability P_{ij} above defined takes the form, $P_{IJ}(l,k)$, where the index l indicates fuel grain f or diluent m in the macroscopic region I and the index k does fuel grain f or diluent m in the macroscopic region J. According to the derivation by Leslie & Jonsson[70], the off-diagonal element of the collision probability is given by

$$P_{IJ}(l,k) = \alpha_{lI}\alpha_{kJ}\frac{W_I}{W_{lI}}P_{IJ} \quad , \tag{7.3.5-3}$$

and the diagonal element by

$$P_{II}(l,k) = Q_I(l,k) - \frac{W_I}{W_{lI}}(1-P_{II})\alpha_{lI}\alpha_{kI} \quad , \tag{7.3.5-4}$$

where $W_{lI} = \Sigma_{lI}V_{lI}$, $W_I = \Sigma_I V_I$ and $\sum_l \alpha_{lI} = 1$,
α_{lI}, Σ_{lI} and V_{lI} are the fraction of collision, the total cross-section and the volume of the region (l in I), respectively, Σ_I and V_I are the corresponding quantities for the macroscopic region I. The quantity $Q_I(l,k)$ is the probability defined to an imaginary infinite lattice consisting of the microscopic cell of the region I, which can be evaluated numerically by the formalism presented in Appendix B of the reference[36] assuming a spherical cell with the white boundary condition. The quantity P_{IJ} denotes the collision probability between macroscopic regions I and J, which is assumed to be obtained using a homogenized cross-section which substitutes for the heterogeneous fuel region.

If we can determine, independently of the macroscopic configuration of I, both of the quantity α_{lI} and the homogeneous-equivalent cross-section Σ_I of the medium I, we can obtain $P_{IJ}(l,k)$ by the following procedure:

Now, we define the self-shielding factor f for the fuel grain so as to give an equivalent collision cross-section to the macroscopic fuel region under the assumption of a uniform flux distribution through the microscopic cell. That is to say, the fraction of collision rate α_l in the region l is assumed to be given by the effective collision cross-section Σ_F and the self-shielding factor f, i.e.,

$$\alpha_f = \frac{V_f\ f\ \Sigma_f}{V_F\Sigma_F} \quad , \tag{7.3.5-5}$$

$$\alpha_m = \frac{V_m\ \Sigma_m}{V_F\Sigma_F} \quad , \tag{7.3.5-6}$$

$$\alpha_f + \alpha_m = 1 \quad , \tag{7.3.5-7}$$

and $V_F = V_f + V_m$,

where Σ_m, is the macroscopic cross-section of the graphite diluent, and V_f and V_m are the volumes of the grain and the associated diluent, respectively. Since we treat only one kind of medium with grain structure, we drop the subscript I for simplicity.

Insertion of Eqs.(7.3.5-5) and (7.3.5-6) into Eq.(7.3.5-7) gives the equivalent cross-sections of the fuel compact, Σ_F as

$$\Sigma_F = \frac{1}{V_F}\left(V_f \; f \; \Sigma_f + V_m \Sigma_m\right) \quad . \tag{7.3.5-8}$$

When one of four variables; f, Σ_F, α_f, or α_{m} is given, then the rest is determined by the relations expressed by Eqs.(7.3.5-5), (7.3.5-6), and (7.3.5-7).

Using the newly defined variables, Eqs.(7.3.5-3) and (7.3.5-4) can be rewritten, respectively, as

$$P_{IJ}(l,k) = f_{lI} \; \alpha_{kJ} \; P_{IJ} \quad , \tag{7.3.5-9}$$

$$P_{II}(l,k) = Q_I(l,k) - f_{lI} \; \alpha_{kl}(1 - P_{II}) \quad , \tag{7.3.5-10}$$

where $f_{lI} = f$ for the fuel grain, and $f_{lI} = 1$ for the diluent.

When the collision probability is given, Eqs.(7.3.5-1) and (7.3.5-2) can be solved recurrently on hyper-fine groups in the dominant resonance energy range, E<130 eV, as described in the last subsection. That is, for computation of neutron flux on a uniform lethargy mesh, we use the RIFF-RAFF method developed by Kier[22), 66)]. Hence, the lethargy mesh Δu used is sufficiently narrow, say Δu =0.00125, compared with the maximum lethargy gain per collision with the heaviest nucleus in the system under consideration. This mesh is also narrow compared with the Doppler width at room temperature. The resonance cross-sections are prepared at the mid-point of each hyper-fine group using a code MCROSS[71)]. The time-consuming computation of collision probabilities for each hyper-fine group is economized using an interpolation scheme, where the values of P_{IJ} are interpolated from the tabulated values on a dozen points of the absorber cross-sections.
We present the following four models for the calculation of the self-shielding factor *f*.

(1) Smearing Method

We assume that the grain medium is made up of an infinite number of microscopic cells and the neutron balance can be described by using the two-region collision probability

$$P_{ij} = Q_I(i, j) \quad . \tag{7.3.5-11}$$

Equations (7.3.5-1) and (7.3.5-2) are solved by following the same procedure as above described. Resonance cross-sections of each resonant nuclide are spatially smeared without collapsing the

hyper-fine groups to give their representative values for the medium. That is, the homogenized cross-section σ_h is obtained by the flux-volume weighted average of the resonance cross-section σ_f, i.e.,

$$\sigma_h(u) = \frac{\sigma_f(u) V_f \varphi_f(u)}{V_f \varphi_f(u) + V_m \varphi_m(u)} \quad .$$

If we define the self-shielding factor f

$$f = \frac{(V_f + V_m)\varphi_f(u)}{V_f \varphi_f(u) + V_m \varphi_m(u)} \tag{7.3.5-12}$$

we can obtain σ_h by a simple volume-weighted average of the effective cross-section, $f\sigma_f$ as

$$\sigma_h(u) = \frac{f\ \sigma_f(u) V_f}{V_f + V_m} \quad .$$

Thus, the effective microscopic cross-section $f\sigma_f$ can be treated as if it is the resonance cross-section of one constituent in a homogeneous medium. The resulted variation of the cross-section with neutron energy is much smooth, compared with the original cross-section, due to the spatial shielding. The shielded cross-sections are prepared for all the reactions of the resonant nuclides under consideration.

(2) Collision Rate Method

As noted before, the fraction of collision rate σl was introduced as to be independent of the origin of neutron. We can suppose several origins of neutron, for example, a neutron just having escaped from the absorber grain, a neutron emitted from the diluent, a neutron impinging on the outer surface of the imaginary cell, or a neutron beam injected into the medium of grain structure, etc.

Now we introduce a quasi-analytic expression of the collision probability for the imaginary cell to give a physical explanation. The following approximation was derived by Nordheim[72]:

$$Q(f, m) = P_e \left[\frac{1 - c}{1 - (1 - l_f \Sigma_f P_e) c} \right] \quad , \tag{7.3.5-13}$$

where P_e (=1-P_c) is the escape probability[27] from an individual grain, c, the Dancoff correction, and Σ_f is the macroscopic cross-section of the absorber grain and its mean chord length l_f is given by

$$l_f = \frac{4V_f}{S_f} \quad , \tag{7.3.5-14}$$

where S_f is the surface area of the absorber grain. The conservation and reciprocity relations give other elements of $Q(l, k)$.

We shall discuss the following two models of neutron origin for calculating the collision rates.

1) Neutron emitted from absorber grain

Segev[73] proposed an expression for the self-shielding factor which was obtained by equating the term in the brackets of Eq.(7.3.5-13) to $[1/(1+fV_f\Sigma_f/V_m\Sigma_m)]$ which is the probability that a neutron escaping from a lump will collide in the diluent of the homogenized medium. The resultant expression is

$$f=\frac{c}{1-c}\frac{V_m\Sigma_m l_f}{V_f}P_e \tag{7.3.5-15}$$

Inserting this expression into Eqs.(7.3.5-5), (7.3.5-6) and (7.3.5-8), we obtain

$$\alpha_f(f)=\frac{l_f\ \Sigma_f\ P_e\ c}{1-(1-l_f\ \Sigma_f\ P_e)\,c}\quad , \tag{7.3.5-16}$$

$$\alpha_m(f)=\frac{1-c}{1-(1-l_f\ \Sigma_f\ P_e)\,c}\quad , \tag{7.3.5-17}$$

where the index (*f*) of $\alpha_f(f)$ denotes that the origin of neutron is fuel grain. It can be explained that the fraction of collision rate is measured for a neutron just having escaped from the absorber grain. That is, the probability that the neutron has the next collision with other grains is given from the expression of Eq.(7.3.5-13)

$$\begin{aligned}Q(f,f)-P_c&=1-Q(f,m)-(1-P_e)\\&=\frac{l_f\Sigma_f P_e^{\,2}\,c}{1-(1-l_f\Sigma_f P_e)\,c}\quad .\end{aligned} \tag{7.3.5-18}$$

On the other hand, the collision with the diluent is given by $Q(f, m)$, which can be calculated by the reciprocity relation. Dividing these quantities by the escape probability P_e, we have the fractions of collision rates; α_f and αm just defined by Eqs.(7.3.5-16) and (7.3.5-17). Inserting Eqs.(7.3.5-16) and (7.3.5-17) into Eqs.(7.3.5-5) and (7.3.5-6), we obtain the same expression of *f* as Eq.(7.3.5-15).

2) Neutron emitted from the diluent

We can define the collision rate for a neutron emitted from the diluent. It is given directly by either $Q(m, f)$ or $Q(m, m)$. A little algebra using the reciprocity relation gives

$$\alpha_f(m)=\frac{V_f\Sigma_f}{V_m\Sigma_m}\frac{P_e\,(1-c)}{1-(1-l_f\Sigma_f P_e)\,c}\quad , \tag{7.3.5-19}$$

where the index *m* of $\alpha_f(m)$ denotes that the origin of neutron is the diluent.

We shall compare the αf 's above introduced. The ratio of $\alpha_f(f)$ to $\alpha_f(m)$ is given by

$$\frac{\alpha_f(f)}{\alpha_f(m)} = \frac{V_m \Sigma_m l_f}{V_f} \frac{c}{1-c} \quad . \tag{7.3.5-20}$$

Lane *et al.*[74] gave a rational expression for the Dancoff correction in case of the small volume fraction of grain by

$$c = 1 \Big/ \left(1 + \frac{V_m \Sigma_m l_f}{V_f} \right) \tag{7.3.5-21}$$

Insertion of Eq.(7.3.5-21) into Eq.(7.3.5-20) gives $\alpha_f(f)/\alpha_f(m) = 1$. This fact means the two models identical in the limited case of the small volume fraction of grain. As shown later numerically, however, $\alpha_f(f)$ always smaller than $\alpha_f(m)$ because the Dancoff correction accurately estimated is slightly lower than the value given by Eq.(7.3.5-20). It can be physically explained: The neutron just having escaped from the absorber grain has to escape from the cell in order to collide with other grains, whereas the neutron emitted from the diluent may collide with the grain in the same cell and also it is at a shorter distance from the grains in the outside of the cell than the former.

Hence, the latter has always the larger probability to collide with the grain than the former has.

Insertion of Eq.(7.3.5-21) into Eq.(7.3.5-15) gives $f=P_e$, then Eq.(7.3.5-8) in this case is given by

$$\Sigma_F = (\nu_f P_e \Sigma_f + \nu_m \Sigma_m) / \nu_F \tag{7.3.5-22}$$

which is just the expression given by Lane *et al.*[74]

The concrete form of P_e by Case *et al.*[27] gives readily the limiting values of Σ_F, i.e.

$$\Sigma_F = \begin{cases} (V_m \Sigma_m + \pi R_f^{\,2}) / V_F & \text{for} \quad R_f \Sigma_f >> 1, \\ (V_m \Sigma_m + V_f \Sigma_f) / V_F & \text{for} \quad R_f \Sigma_f << 1, \end{cases} \tag{7.3.5-23}$$

where R_f is the radius of the absorber grain. Here, it should be noted that the effective cross-section, Σ_F is bounded to be finite even if Σ_F goes to infinite. This behavior is an essential feature of the grain effect.

(3) Transmission Cross-section Method

Supposing the attenuation of a uniform current of neutron beam through a media having grain structure, Tsuchihashi & Gotoh[36] presented a formulation of the equivalent cross-section, Σ_F given by the solution of a following transcendental equation:

$$X \exp(-X) = C \quad , \tag{7.3.5-24}$$

where

$$X = 2R_p(\Sigma_F - \Sigma_m) \quad ,$$
$$C = 2R_p \pi\rho R_f{}^2 \, F\{2R_f(\Sigma_f - \Sigma_m)\} \quad ,$$
$$F(x) = 1 - 2\{1 - (1+x)\exp(-x)\}/x^2 \quad ,$$

R_p, the radius of the coated particle, and ρ is the number density of particles. The equivalent cross-section corresponds to the smaller root of Eq.(7.3.5-24), and is always slightly larger than $\Sigma_m + C/2R_p$.

If account is taken of the fact that $F(x)$ is a monotonously increasing function for $x > 0$ and

$$F(x) = \begin{cases} \frac{2}{3}x + O(x^2) & \text{for } |x| << 1 \quad , \\ 1 + O(x^{-2}) & \text{for } x >> 1 \quad . \end{cases} \tag{7.3.5-25}$$

we can show that Eq.(7.3.5-24) has the proper limit values for the black limit ($R_f\Sigma_f >> 1$) and the homogeneous limit ($|(\Sigma_f - \Sigma_m)R_f| << 1$) just the same as given in Eq.(7.3.5-23).

We have not described yet the treatment of the double heterogeneity in the higher resonance energy range; say: $E > 130$ eV. We take the table-look-up method for the resonance shielding factors. We adopted Segev's expression[73] based on the NR approximation for the background cross-section presenting the heterogeneous effect, i.e.,

$$\Sigma_e = \frac{1-c}{l_f} \frac{a}{1 + c\,(a\beta - 1)} \quad , \tag{7.3.5-26}$$

and

$$\beta = \frac{V_m / V_F}{V_m / V_F + (1-C)A / L(1 + C(A-1))} \quad , \tag{7.3.5-27}$$

where a and A are the Bell or Levine factor for the microscopic and macroscopic cells, respectively, and C and L are the Dancoff correction and the mean chord length of the macroscopic cell, respectively.

The above treatment is incorporated into the SRAC code system together with the models described above for the lower energy range, to yield the resonance absorption in a doubly heterogeneous cell.

A sequence of study using the present method gives us confidence that the present approach is straightforwardly applicable to the doubly heterogeneous system with the realistic geometry such as LWR and LMFBR lattice cells since our treatment on the macroscopic geometry is fairly general. This method allowing three one-dimensional (sphere, plane and cylinder) cells as optional microscopic geometry has been incorporated in the SRAC code system.

7.4 Solution of Linear Equation

It is one of the features of the SRAC code system to execute the cell calculations by the collision probability method to cover the whole neutron energy range. In this section we shall describe how to solve the linear equation introduced in Sect.7.1.

Because of the difference of physical characteristics, the different specialized equation is formulated separately by neutron energy range. Although the concatenation of the equations into a set of equations so as to describe the quantities in the whole neutron energy is available, the cell calculation is usually achieved separately by neutron energy range. Partly because there occurs no up-scattering in the epi-thermal and fast neutron energy range, but does in the thermal neutron range where any iterative process among the energy group variables is required. Partly because the neutron flux distribution in the fast and epi-thermal neutron range is relatively flat, which allows coarse spatial division of the cell model or the overall flat flux assumption coupled with some suitable resonance shielding treatments. However, the distribution in the thermal neutron range shows sharp spatial change due to small flight path. In this energy range needs fine spatial division. It is to be noted that although there occurs the sharp flux depression due to the strong resonance structure of the fertile nuclides near the resonance energy, fine spatial division is not necessary to evaluate the overall resonance absorption. Because neutrons scarcely come out from the place where the depression occurs, the shape of the depression does not affect the absorption rate.

7.4.1 General Form of Linear Equation

When the system under consideration is divided into *N* regions and the neutron energy range is divided into *G* groups, Eq.(7.1-9) is rewritten as

$$\Sigma_{jg}\varphi_{jg} = \sum_{i=1}^{N} P_{ijg}\left\{\sum_{g'=1}^{G}\Sigma_{sig'\to g}\varphi_{ig'} + S_{ig}\right\} \tag{7.4.1-1}$$

The physical quantities are redefined as follows:

- the volume of the region *i*; $V_i = \int_{V_i} dV$
- the integral flux over the region *i* for the energy group *g*;

$$\varphi_{ig} = \int_{V_i} dV \int_{\Delta E_g} dE\ \varphi(\mathbf{r}, E)$$

- the fixed source; $S_{ig} = \int_{V_i} dV \int_{\Delta E_g} dE\ S(\mathbf{r}, E)$
- the collision probability from the region *i* to *j* for the group *g*; P_{ijg}

- the reduced collision probability which has finite value even if the collision region *j* is vacuum; $P^{\#}{}_{ijg} = P_{ijg} / \Sigma_{jg}$

- the emission rate of the region *i* for the group *g*; H_{ig}

- Nuclear constants of the material *m*;

  Σ_{mg} = total cross-section,

  $\nu\Sigma_{fmg}$ = production cross-section,

  Σ_{amg} = absorption cross-section,

  $\Sigma_{smg'\to g}$ = scattering cross-section from the group g' to the group g

  $\Sigma_{rmg} = \sum_{g'\notin G} \Sigma_{smg\to g'} + \sum_{g'\notin G} \chi_{mg'} \nu\Sigma_{fmg}$,

  scattering-out cross-section which is used to evaluate the neutron balance of the system. It has non-zero value when a fixed source problem of a limited energy range is considered. The quantity χ_{mg} stands for the fission yield to the group *g*.

Using the above definitions, the equation to be solved is written by

$$\varphi_{ig} = \sum_{j} P^{\#}{}_{jig} H_{jg} \tag{7.4.1-2}$$

The emission rate for the fixed source problem is written by

$$H_{ig} = S_{ig} + \sum_{g'=1}^{G} \Sigma_{smg'\to g} \varphi_{ig'} \quad + \quad \chi_{mg} \sum_{g'=1}^{G} \nu\Sigma_{fmg'} \varphi_{ig'} \tag{7.4.1-3a}$$

where *m* denotes the material assigned to the region *i*.
For the eigenvalue problem,

$$H_{ig} = \sum_{g'=1}^{G} \Sigma_{smg'\to g} \varphi_{ig'} \quad + \quad \frac{\chi_{mg}}{\lambda} \sum_{g'=1}^{G} \nu\Sigma_{fmg'} \varphi_{ig'} \tag{7.4.1-3b}$$

Equation (7.4.1-2) coupled with Eq.(7.4.1-3a) forms inhomogeneous equations and that coupled with the Eq.(7.4.1-3b) forms homogeneous equations. In both problems, the number of unknown is *N***G*. The general matrix of the same rank consists of $(N*G)^2$ elements, however, the computer storage required for the above equations is at most ($N^2G+MG^2 < NG(N+G)$: (N^2G) for the collision probability and (MG^2) for scattering matrix, where *M* is the number of materials. The size (G^2) for the scattering

matrix will be reduced if only down-scattering is considered or only heavy nuclides compose a material. In the following sections the techniques to reduce the computer time and storage for several particular problems will be described.

7.4.2 Iterative Procedure in Thermal Energy Range

In the thermal neutron energy range, the emission rate Eq.(7.4.1-3a) is rewritten as

$$H_{ig} = S_{ig} + \sum_{g'=1}^{G} \Sigma_{smg' \to g} \varphi_{ig'} \tag{7.4.2-1}$$

The fixed source S_{ig} is usually given by the slowing-down from the epi-thermal range. Since the fluxes are completely coupled each other by up- and down-scattering, the equations of the form of Eq.(7.4.1-2) and (7.4.2-1) are solved by an iterative procedure by using the method of Successive Over Relaxation (SOR) as used in the THERMOS Code[34]. Some extension was made to consider an isolated cell and the outer iteration for the eigenvalue problem to the original routine. The procedure is as follows;

Step 1. Set the initial guess of φ_{ig}

Step 2. Obtain the normalization factor for the source term,

$$B = \sum_{g=1}^{G} \sum_{i=1}^{N} S_{ig} \sum_{j=1}^{N} P_{ijg} \quad .$$

After finding B, every S_{ig} is divided by B. Thus the total number of neutrons which will have the next collision in the system considered is set to unity.

Step 3. Calculate H_{ig} according to Eq.(7.4.2-1) and simultaneously the scaling factor C;

$$C = \sum_{g=1}^{G} \sum_{j=1}^{N} \left\{ \Sigma_{mg} \varphi_{ig} - (H_{ig} - S_{ig}) \sum_{j=1}^{N} P_{ijg} \right\} \quad ,$$

which is defined as the ratio of the removal reaction (absorption, scattering-up above the thermal cut off energy, and leakage) to the source which will have the next collision in the system. This factor must be unity in the converged state.

Step 4. Calculate the new fluxes $\varphi^{(m+1/2)}$ according to Eq.(7.4.1-2) and the weighted residual,

$$R^{(m)} = \left\{ \sum_{g=1}^{G} \sum_{i=1}^{N} \left(\varphi_{ig}^{(m+1/2)} / C - \varphi_{ig}^{(m)} \right)^2 R_{ig}^2 \Big/ \sum_{g=1}^{G} \sum_{i=1}^{N} R_{ig}^2 \right\}^{1/2} \quad .$$

The root mean square (RMS) residual will be used to estimate the converging slope as $\mu^{(m)} = R^{(m)} / R^{(m-1)}$. The weighting reaction R_{ig} is fixed to absorption $\Sigma_a \varphi_{ig}$. The superscript (m) is an iteration counter.

Step 5. Modify the over-relaxation factor ω. In the first L_e iterations, the initial value of ω_0 will be used. At each iteration, the value of ω_e=1/(1-$\mu^{(m)}$) is tested. If all the values of ω_e in the last L_e iterations agree within the given extrapolation criterion ε_e, an extrapolation takes place using the most recent value of ω_e. The testing for a possible extrapolation is suppressed during the L_d iterations following the extrapolation. The value λ (the estimate of the eigenvalue of the matrix considered) is computed as λ=($\mu^{(m)}$-1+ω_0) and a new ω is obtained as ω_1 = 2/(2-λ) to be used after the next iteration.

If an increase of the residual is detected during the iteration, a moderate value of ω is selected as

$$\omega_2 = (\omega_1 \times f_{under})^{1/2} \quad .$$

Step 6. Obtain the new fluxes by the over-relaxation;

$$\varphi_{ig}^{(m+1)} = \varphi_{ig}^{(m)} + \omega\left(\varphi_{ig}^{(m+1/2)} / C - \varphi_{ig}^{(m)}\right) \quad .$$

The loop from Step 3 to Step 6 is repeated until the residual $R^{(m)}$ is less than ε_e or the iteration counter m exceeds L_{in}. The quantities ε, ω_0, ε_e, f_{under}, L_e, L_d, and L_{in} are input numbers.

In the practical use of this procedure, we find that the scaling by C is effective to accelerate the convergence, but, we encounter some difficulties in attaining the convergence. One problem occurs in a weakly absorbing case where a slow convergence rate is observed through the iteration. Once an extrapolation is taken place, while it greatly reduces the RMS residual, the new over-relaxation factor ω_1 which takes the value close to 2.0, say, 1.8 after the extrapolation, causes growth of the residual in most cases. The following procedure which is activated when the increase of the residual is detected in order to have a moderate over-relaxation factor ω_2 helps to escape from such a catastrophe. Another problem happens in a strongly absorbing case where we encounter also growth of the residual. It is the case in which we can expect a rapid convergence. It is thought that because the secondary eigenvalue of the matrix, λ is not far from the largest eigenvalue λ_0, the spectral radius of the higher mode in the modified matrix might exceed unity. We can escape from this trouble by feeding a relatively low f_{under}, say 0.5, which suppresses the new factor ω_2 below unity. In other word, in a strongly absorbing case, an under-relaxation is required.

As the computer time required for the iterative process is much shorter than that for the preparation of collision probabilities, the optimum use of the above procedure is not essential. We may suppress the extrapolation by feeding the strict criterion ε_e not to activate the extrapolation. Against the case where the divergence may occur, the low value of f_{under} can prevent the divergence.

7.4.3 Solution by Matrix Inversion in Fast Neutron Range

For the fixed source problem in the fast neutron range, the emission rate can be rewritten by

$$H_{ig} = S_{ig} + \sum_{g'=1}^{g} \Sigma_{smg' \to g} \varphi_{ig'} + \chi_{mg} \sum_{g'=1}^{G} \nu\Sigma_{fmg'} \varphi_{ig'} \quad . \tag{7.4.3-1}$$

The fixed source term S_{ig} usually consists of the thermal fission neutron. The scattering term is determined by the fluxes of the upper energy groups. Given the fast fission term, the fluxes can be successively solved starting at the highest energy group. The number of the unknowns to be simultaneously solved is the total number of regions, N.

We have a choice for the solution whether by an iterative method or by a matrix inversion. As far as N is less than about 40, the round-off error due to the limited computer precision encountered in the matrix inversion can be negligible. The computer time required for the matrix inversion (proportional to N^3) does not so much exceed that for the iterative method (proportional to the iteration count*N^2). In the SRAC code system, the matrix inversion is applied preferring its definitive solution.

After finding the flux distribution for all the energy groups, we have to modify the assumed fast fission source distribution by an iterative process. This power iteration converges rapidly for the case of a thermal reactor because the ratio of fast fission to thermal fission is small. Contrary, the procedure of this section can not be applied for the fast reactor where the matrix may have an eigenvalue greater than unity.

The procedure described in this section is summarized as follows;

Step 1. Normalize the fixed source S_{ig}.

Step 2. Set the initial guess for the fast fission distribution.

Step 3. Starting at the highest energy group g=1, calculate emission rates of a group H_{ig} by Eq.(7.4.3-1).
Calculate fluxes of a group by a matrix inversion.
Repeat Step 3 for all groups.

Step 4. Calculate fast fission distributions and modify it by an SOR.

Repeat Step 3 and 4, until the fast fission distribution converges.

7.4.4 Iterative Procedure for Eigenvalue Problem in Whole Energy Range

Considering the fact that while the iteration count in the thermal energy range amounts to several tens, in the fast energy range any iterative process is not needed, the treatment for the thermal

group flux and for the fast group flux should be different when both have to be solved simultaneously in the whole energy range.

Our scenario to solve the eigenvalue problem in the whole energy range in the cell calculation is a combination of the procedures described in the previous two sections, as follows;

Step 1. Set an initial guess of fission distribution and normalize it.

Step 2. Starting at the highest energy group g=1, calculate the emission rate of a group H_{ig} by Eq.(7.4.3-1).
Calculate fluxes of a group by a matrix inversion.
Repeat Step 2 for all fast groups.

Step 3. Calculate the slowing-down source to the thermal groups.

Step 4. Calculate the thermal fluxes by repeating the thermal iteration as described in Sect.7.4.1 until the convergence is attained or the fixed iteration count is reached.

Step 5. Calculate and re-normalize the fission distribution using the new flux distribution and modify the distribution by an SOR.

Repeat Step 2 through Step 5 until the fission distribution converges. The eigenvalue is obtained as the re-normalization factor of fission distribution calculated in Step 5 at the final power iteration.

7.5 Smearing and Collapsing of Group Constants

It is one of the features of the SRAC code system to execute smearing and collapsing in separate steps and for the user to control the timing. The smeared cross-sections can be used by the succeeding cell calculation in the case of double heterogeneity. Smearing may be done by using the spatial distribution of the fluxes obtained by the cell calculation, over a whole cell or on partitioned regions which are specified by X-Region. Description will be also made for the optional calculation of cell averaged diffusion coefficient specified by IC17 in Sect.2.2.

Next, discussions will be made on the optional use of neutron spectrum for collapsing, as we have several choices, as follows;

(a) the asymptotic spectrum characterized by Maxwellian temperature stored in FASTU and THERMALU files
(b) the spectrum to a mixture provided by the user in FLUX file,
(c) the spectrum calculated by P_1 or B_1 approximation to an isolated mixture specified by IC16 which was used for the transport cross-sections of the mixture,
(d) the spatially integrated spectrum of the flux obtained by the cell calculation,
(e) if the above is for an infinite array of lattice cell, the spectrum recalculated by the P_1 or B_1 approximation activated by IC9 to include the leakage effect, where attention is paid to reflect this leakage correction on the space-dependent spectrum order to give the suitable reaction rate of depleting nuclide associated to the mixture to cell burn-up routine.

Collapsing of energy group structure for few group core calculation is described with emphasis on the diffusion parameter.

Description will be given using the following nomenclature.

Table 7.5-1 (1/2) Nomenclature

Symbols	Meaning
g , g'	Multi-group number
G , G'	Few group number
i , j	A) In the collision probability method: T- or R-Region number, which is used as spatial index. B) For S_N and diffusion calculation: fine mesh number
m	Material number for spatial region i or j, in other words, m-th M-Region which includes regions i or j.
I	X-Region number for editing region to which the average cross-section is given (usually I =1 is given throughout the system, except for the case where a super-cell model is used.)
(*Note* : $i, j \in m \in I$)	
z	Nuclear reaction for process z (fission, capture, scattering, etc.)
n	Nuclide.
l	Order of Legendre expansion (l =0 or 1).
$\chi_{g,m}$	Fission spectrum of material m.
$\sigma^{n}_{z,m,g}$	Effective multi-group cross-section of nuclide n in material m (z = fission or capture), which is obtained by the interpolation of the self-shielding factors stored in FASTU and THERMALU files except for the resonance energy range II where hyper-fine group calculation or IR method can be used. This cross-section is kept in MICREF file in order to be used for cell burn-up calculation or for activation calculation.
$\sigma^{n}_{z,m,G}$	Effective few-group cross-section of nuclide n in material m (z = fission or capture) given to the cell burn-up routine but not kept.

Table 7.5-1 (2/2) Nomenclature

Symbols	Meaning
$\Sigma_{z,m,g}$, $\nu\Sigma_{f,m,g}$	Macroscopic multi-group cross-section of material *m*.
$\Sigma_{tr,m,g}$	Macroscopic transport cross-section of material *m*.
$\Sigma_{sl,m,g\to g'}$	Macroscopic energy transfer cross-section of material *m*.
$\overline{\Sigma}_{z,I,g}$, $\nu\overline{\Sigma}_{f,I,g}$	Averaged multi-group cross-section of *I*-th X-Region. Usually one X-Region is assigned to each lattice cell unless a super-cell model is used.
$\overline{\Sigma}_{s0,I,g\to g'}$	Averaged energy transfer cross-section of *I*-th X-Region.
$\overline{\Sigma}_{tr,I,g}$	Averaged transport cross-section of *I*-th X-Region
$\overline{D}_{I,g}$	Averaged diffusion coefficient
$\overline{\chi}_{I,G}$	Few group fission spectrum
$\overline{\Sigma}_{z,I,G}$, $\nu\overline{\Sigma}_{f,I,G}$	Few group cross-section of *I*-th X-Region.
$\overline{\Sigma}_{s0,I,G\to G'}$	Few group energy transfer cross-section of *I*-th X-Region.
$\overline{\Sigma}_{tr,I,G}$	Few group transport cross-section.
$\overline{D}_{I,G}$	Few group diffusion coefficient.
$\varphi_g(\boldsymbol{r}) = \int_{\Delta u_g} \varphi(\boldsymbol{r},u)du$	Analytical expression of space dependent flux of group *g*.
$\varphi_{i,g} = \int_{V_i} \varphi_g(\boldsymbol{r})d\boldsymbol{r} / V_i$	Average flux of region *i* and integrated in group *g*.
$\overline{\Phi}_{m,g} = \sum_{i\in m} \varphi_{i,g}V_i / V_m$	Average flux of region *m* of multi-group *g*.
$\overline{\Phi}_{m,G} = \sum_{g\in G} \overline{\Phi}_{m,g}$	Average flux of region *m* of few-group *G*.
$\overline{\Phi}_{I,g} = \sum_{i\in I} \varphi_{i,g}V_i / V_I$	Average flux of region *I* of multi-group *g*.
$\overline{\Phi}_{g} = \sum_{i\in cell} \varphi_{i,g}V_i / V_{cell}$	Average flux of whole cell of multi-group *g*.
$\overline{\Phi}_{I,G} = \sum_{g\in G} \overline{\Phi}_{I,g}$	Average flux of region *I* of few-group *G*.

7.5.1 Smearing

Smearing or spatial average of cross-sections is achieved in the MIXX routine by using the spatial distribution of the flux $\varphi_{i,g}$ obtained by the cell calculation as described in Sect.7.4.

When the second resonance energy range below 130.07eV (or 961.12eV) is treated by the direct method described in Sect.7.3 using the PEACO routine, the effective cross-sections in each region and the fluxes with multi-group structure obtained by Eq.(7.4.1-1) are replaced by those from the PEACO routine.

$$\overline{\Sigma}_{z,I,g} = \sum_{i\in I} \Sigma_{z,m,g} V_i \varphi_{i,g} \Big/ (\overline{\Phi}_{I,g} V_I) \tag{7.5-1}$$

$$\overline{\nu\Sigma}_{f,m,g} = \sum_{i\in I} \nu\Sigma_{f,m,g} V_i \varphi_{i,g} \Big/ (\overline{\Phi}_{I,g} V_I) \tag{7.5-2}$$

$$\overline{\chi}_{I,g} = \sum_{i\in I} \chi_{m,g} \sum_{g'} \nu\Sigma_{f,m,g'} V_i \varphi_{i,g'} \Big/ \sum_{i\in I} \sum_{g'} \nu\Sigma_{f,m,g'} V_i \varphi_{i,g'} \tag{7.5-3}$$

$$\overline{\Sigma}_{sl,I,g\to g'} = \sum_{i\in I} \Sigma_{sl,m,g\to g'} V_i \varphi_{i,g} \Big/ (\overline{\Phi}_{I,g} V_I) \tag{7.5-4}$$

Benoist presented a theory of the diffusion coefficient in reactor lattice, leading to expressions valid in full generality[25]. For the diffusion coefficient of the direction *k*, omitting the absorption correction and angular terms, this theory gives

$$\overline{D}_{k,g} = \sum_i \sum_j V_i \varphi_{i,g} \lambda_{j,g} P_{ijk,g} \Big/ (3\sum_i V_i \varphi_{i,g}) \quad . \tag{7.5-5}$$

where *i* and *j* stand for the region number, $\lambda_{j,g}$ the transport mean free path for region *j* given by $1/\Sigma_{tr,m,g}$ and $P_{ijk,g}$ is a directional first flight collision probability given by Eq.(7.1-16).

Three options are provided for calculating the diffusion coefficient $\overline{D}_{k,g}$.

(1) Optional Process IC17 = 1

The first option is a rather sophisticated one which has been proven by experience to be fairly accurate, and the diffusion coefficient is given by the inverse of the cell averaged transport cross-section, i.e.,

$$\overline{D}_{h,g} = \sum_i V_i \varphi_{i,g} \Big/ (3\sum_i V_i \varphi_{i,g} \Sigma_{tr,m,g)} \, . \tag{7.5-6}$$

When the flux $\varphi_{i,g}$ are flat in the whole system and we can assume

$$P_{ijk,g} = V_i \Sigma_{tr,m,g} \Big/ (\sum_j V_j \Sigma_{tr,m,g}) \qquad \text{(homogeneous limit)} \tag{7.5-7}$$

independent of *k*, we have

$$\overline{D}_{h,g} = \sum_i V_i \Big/ (3\sum_i V_i \Sigma_{tr,m,g}) . \tag{7.5-8}$$

Contrary, if a neutron born in any region *i* is certain to suffer its first collision in this region (the assumption that each region is large compared to the mean free path), then

$$P_{ijk,g} = \delta_{ij} \tag{7.5-9}$$

and

$$\overline{D}_{t,g} = \sum_i V_i \varphi_{i,g} \lambda_{i,g} \Big/ (3\sum_i V_i \varphi_{i,g}) . \tag{7.5-10}$$

It follows at once from the fundamental theorem of algebra

$$\overline{D}_{t,g} \geq \overline{D}_{h,g} . \tag{7.5-11}$$

The use of $\overline{D}_{t,g}$ to the cell with voided regions falls into the drawback that the diffusion coefficient is unreasonably large to be used in practical calculation.

(2) Optional Process IC17 = 2

The isotropic diffusion coefficient is used and defined by

$$\overline{D}_{0,g} = \frac{1}{3} \sum_k D_{k,g} . \tag{7.5-12}$$

Then, from the definition of the directional collision probability by Eq.(7.1-16), this diffusion coefficient can be calculated using the isotropic collision probability defined by Eq.(7.1-13), i.e.,

$$\overline{D}_{0,g} = \sum_i \sum_j V_i \varphi_{i,g} \lambda_{j,g} P_{ij,g} / (3\sum_i V_i \varphi_{i,g}) \tag{7.5-13}$$

(3) Optional Process IC17 = 3

The anisotropic diffusion coefficients defined by Eq.(7.5-5) are calculated. These coefficients are used for the 2-D or 3-D diffusion calculation using the CITATION code.

7.5.2 Spectrum for Collapsing

The fluxes thus used are however not taken account of the neutron leakage from the system under study. So these fluxes should be renormalized to take account of the leakage. For this purpose, the homogenized effective cross-sections are at first calculated without any group collapsing for the whole energy range to obtain the homogeneous P_1 or B_1 spectrum.

The P_1 or B_1 equation in multigroup form can be written in the conventional and unified way as

$$\begin{aligned} F_{1,g} + \overline{\Sigma}_{tg} F_{0g} &= \sum_{g'=1}^{G} \overline{\Sigma}_{s0g'\to g} F_{0g'} + \overline{\mathrm{X}}_{0g} \quad , \\ 3\alpha_g \overline{\Sigma}_{t,g} F_{1g} - B^2 F_{0g} &= \sum_{g'=1}^{G} \overline{\Sigma}_{s1g'\to g} F_{1g'} \end{aligned} \tag{7.5-14}$$

where α_g equals unity for the P_1 approximation and is given for the B_1 approximation by

$$\begin{aligned} \alpha_g &= (x_g \tan^{-1} x_g) \Big/ 3\left\{1 - (\tan^{-1} x_g)/x_g\right\} \qquad \text{for} \quad B^2 \geq 0 \\ \alpha_g &= (x_g \tanh^{-1} x_g) \Big/ 3\left\{1 - (\tanh^{-1} x_g)/x_g\right\} \qquad \text{for} \quad B^2 \leq 0 \end{aligned} \tag{7.5-15}$$

with $\quad x_g = \sqrt{|B^2|} \Big/ \overline{\Sigma}_{t,g}$,

where the quantity B^2 is the value entered in Block-4 of Sect.2.2.

Assuming a fission spectrum as the source term. Eq.(7.5-2) is solved by the P_1 or B_1 approximation for the fast energy range, while the solution is obtained in the thermal energy range assuming a slowing-down source. The linked spectrum for the whole energy range is optionally used to replace the spectrum of the flux of the cell calculation obtained by assuming an infinite array of lattice cell.

Using the solution, $\varphi_{i,g}$, of Eq.(7.4.1-1), the spatially averaged fluxes are calculated by

$$\overline{\Phi}_g = \sum_{i \in cell} V_i \varphi_{i,g} / V_{cell} \ . \tag{7.5-16}$$

Then, the spectrum which includes the leakage effect can be given by

$$\varphi'_{i,g} = \varphi_{i,g} F_{0g} / \overline{\Phi}_g \, . \tag{7.5-17}$$

The resultant spectrum $\varphi'_{i,g}$ replaces the infinite spectrum $\varphi_{i,g}$, if the minus sign of IC9 is entered, and is used to give the microscopic effective cross-section $\sigma^{n}_{z,m,G}$ to the cell burn-up routine. Above procedure is executed in the HOMOSP routine.

For the isolated mixture which is not used in the cell calculation, either of the spectra on the items (a), (b) and (c) in the second paragraph of Sec.7.5 will be chosen for the weight.

7.5.3 Collapsing of Group Constants

Collapsed group cross-sections for the few group calculations are obtained from the following prescriptions. Description will be also given for the transport cross-section and diffusion coefficient in the next subsection.

$$\sigma^n_{z,m,G} = \sum_{g\in G} \sigma^n_{z,m,g} \overline{\Phi}_{m,g} \,/\, \overline{\Phi}_{m,G} \quad (z = f \text{ or } c) \tag{7.5-18}$$

$$\overline{\chi}_{I,G} = \sum_{g\in G} \overline{\chi}_{I,g} \tag{7.5-19}$$

$$\overline{\Sigma}_{z,I,G} = \sum_{g\in G} \overline{\Sigma}_{z,I,g} \overline{\Phi}_{I,g} \,/\, \overline{\Phi}_{I,G} \tag{7.5-20}$$

$$\overline{\nu\Sigma}_{f,I,G} = \sum_{g\in G} \overline{\nu\Sigma}_{f,I,g} \overline{\Phi}_{I,g} \,/\, \overline{\Phi}_{I,G} \tag{7.5-21}$$

$$\overline{\Sigma}_{s0,I,G\to G'} = \sum_{g\in G} \sum_{g'\in G'} \overline{\Sigma}_{s0,I,g\to g'} \overline{\Phi}_{I,g} \,/\, \overline{\Phi}_{I,G} \tag{7.5-22}$$

Here the multi-group diffusion coefficients are assumed for each homogenized X-Region (zone).

The group-dependent diffusion equation in the *I*-th region can be written as

$$-\overline{D}_{I,g}\nabla^2\Phi_g(\boldsymbol{r}) + \overline{\Sigma}_{t,I,g}\Phi_g(\boldsymbol{r}) = S_g(\boldsymbol{r}).$$

Let us sum up the above equation over g to collapse the multi-group equation into the few groups and denote each few group by *G*, then we have for the diffusion term

$$-\sum_{g\in G} \overline{D}_{I,g}\nabla^2\varphi_g \approx B^2 \sum_{g\in G} \overline{D}_{I,g}\varphi_g(r) = B^2 \overline{D}_{I,G}\overline{\Phi}_{I,G} \approx -\overline{D}_{I,G}\nabla^2\overline{\Phi}_{I,G}$$

where

$$\overline{\Phi}_{I,G} \equiv \sum_{g\in G} \overline{\Phi}_{I,g} \tag{7.5-23}$$

and

$$\overline{D}_{I,G} \equiv \sum_{g\in G} \overline{D}_{I,g} \overline{\Phi}_{I,g} \,/\, \overline{\Phi}_{I,G}\,. \tag{7.5-24}$$

Hence, the few group transport cross-sections can be defined by

$$\overline{\Sigma}_{tr,I,G} = 3\overline{\Phi}_{I,G} \Big/ \sum_{g\in G} \overline{D}_{I,g} \overline{\Phi}_{I,g} = \overline{\Phi}_{I,G} \Big/ \sum_{g\in G} \frac{\overline{\Phi}_{I,g}}{\overline{\Sigma}_{tr,I,g}}\,. \tag{7.5-25}$$

Here, an equivalent relation holds as

$$\overline{\Sigma}_{tr,I,G} = \frac{1}{3\overline{D}_{h,I,G}} \tag{7.5-26}$$

For the isolated mixture which is not used in the cell calculation, by using either of the spectra on the items (a), (b) and (c) in the second paragraph of Sec.7.5, the procedure mentioned above is taken.

A special treatment is available for a strongly absorbing material where the diffusion equation does not hold, if IC17= -1 is entered by

$$\overline{\Sigma}_{tr,I,G} = \sum_{g\in G} \overline{\Sigma}_{tr,I,g} \overline{\Phi}_{I,g} / \overline{\Phi}_{I,G} \tag{7.5-27}$$

The selection of the definition by IC17 results in the SRAC macroscopic format as shown in Table 7.5-1.

Table 7.5-1 Selection of diffusion coefficient by IC17

IC17	$\overline{\Sigma}_{total}$		D1		D2	
1	$\overline{\Sigma}_{tr,I,g}$	25*	$\overline{D}_{h,g}$	24	$\overline{D}_{t,g}$	24
2	$\overline{\Sigma}_{tr,I,g}$	25	$\overline{D}_{0,g}$	24	$\overline{D}_{t,g}$	24
3	$\overline{\Sigma}_{tr,I,g}$	25	$\overline{D}_{radial,g}$ or $\overline{D}_{\perp,g}$	24	$\overline{D}_{axial,g}$ or $\overline{D}_{\parallel,g}$	24
-1	$\overline{\Sigma}_{tr,I,g}$	27	$\overline{D}_{h,g}$	24	$\overline{D}_{t,g}$	24

Note * Number following the definition denotes the equation number in this section to show how to collapse the quantity into the few group constant.

7.6 Reactivity Calculation by Perturbation Theory

The perturbation theory is used to estimate a small reactivity. Although the CITATION code is a module code in the SRAC code system, the function installed in the original code[6] has not been utilized since it requires the microscopic cross-sections which are not provided in the SRAC code system.

A new routine is made to feed the macroscopic cross-sections into the first order perturbation calculation. The forward and adjoint fluxes have to be prepared by the installed CITATION module. A perturbed region can be specified by the following three modes;

(a) A whole volume specified by a zone number,

(b) A volume specified by mesh numbers of boundaries,

(c) A volume expressed by abscissa of boundaries, and several volumes can be simultaneously accepted in a case. As shown in the input specification in Sect.2.8, a mixed mode of (b) and (c) accepted.

By specifying a new mixture to replace the original mixture located at the perturbed region, the change is automatically calculated from the difference of cross-sections of two mixtures.

The following results will be printed;

- The macroscopic cross-sections of the new mixture.
- The volume of the perturbed region and that of the zone including the region.
- The whole reactivity change, reactivity changes by reaction and by energy group, and their fractions to the whole.
- The reactivity due to the change of leakage on each outer surface and by energy group.
- The summation over total perturbed regions

The following restrictions have to be noted.

- A perturbed region can not extend over two zones. If necessary, a region should be split into two regions.
- When the geometry is 3D triangular or 3D hexagonal, the region specification by abscissa is accepted only in Z-direction.

7.6.1 First Order Perturbation

The reactivity change ρ ($\Delta k/kk'$) by the first order perturbation theory is given by

$$\rho = \frac{\Delta F - \Delta A + \Delta S - \Delta L - \Delta DB^2}{F} \tag{7.6-1}$$

where F is the total fission, ΔF the fission term, ΔA the absorption term, ΔS the scattering term, ΔL the leakage term, ΔDB^2 the pseudo leakage term. These are given by

$$F = \frac{1}{K}\sum_{g}\int \chi_g(\boldsymbol{r})\varphi_g^*(\boldsymbol{r})\sum_{g'}\nu\Sigma_{f\,g'}(\boldsymbol{r})\varphi_{g'}(\boldsymbol{r})dV \tag{7.6-2}$$

where $K = k_{eff}^{p} \approx k_{eff}$ (because of the 1st order perturbation)

$$\Delta F_g = \frac{1}{K}\int \varphi_g^*(\boldsymbol{r})\sum_{g'}\left\{\chi_g(\boldsymbol{r})\Delta\nu\Sigma_{f\,g'}(\boldsymbol{r}) + \Delta\chi_g(\boldsymbol{r})\nu\Sigma_{f\,g'}(\boldsymbol{r})\right\}\varphi_{g'}(\boldsymbol{r})dV \tag{7.6-3}$$

$$\Delta A_g = \int \varphi_g^*(\boldsymbol{r})\Delta\Sigma_{a\,g}(\boldsymbol{r})\varphi_g(\boldsymbol{r})dV \tag{7.6-4}$$

$$\Delta S_g = \int \sum_{g'}(\varphi_{g'}^*(\boldsymbol{r}) - \varphi_g^*(\boldsymbol{r}))\Delta\Sigma_{s\,g'\to g}(\boldsymbol{r})\varphi_{g'}(\boldsymbol{r})dV \tag{7.6-5}$$

$$\begin{aligned}\Delta L_g &= \int \nabla\varphi_g^*(\boldsymbol{r})\Delta D_g(\boldsymbol{r})\nabla\varphi_g(\boldsymbol{r})dV \\ &= \int\left[\left\{\frac{\partial\varphi_g^*(\boldsymbol{r})}{\partial x}\Delta D_{x\,g}(\boldsymbol{r})\frac{\partial\varphi_g(\boldsymbol{r})}{\partial x}\right\} + \left\{\frac{\partial\varphi_g^*(\boldsymbol{r})}{\partial y}\Delta D_{y\,g}(\boldsymbol{r})\frac{\partial\varphi_g(\boldsymbol{r})}{\partial y}\right\}\right. \\ &\quad \left. + \left\{\frac{\partial\varphi_g^*(\boldsymbol{r})}{\partial z}\Delta D_{z\,g}(\boldsymbol{r})\frac{\partial\varphi_g(\boldsymbol{r})}{\partial z}\right\}\right]dV\end{aligned} \tag{7.6-6}$$

$$\Delta DB_g^2 = \int \varphi_g^*(\boldsymbol{r})\left\{\Delta D_{z\,g}(\boldsymbol{r})B_g^2(\boldsymbol{r}) + D_{z\,g}(\boldsymbol{r})\Delta B_g^2(\boldsymbol{r})\right\}\varphi_g(\boldsymbol{r})dV \tag{7.6-7}$$

$$\Delta F = \sum_g \Delta F_g \tag{7.6-8}$$

$$\Delta A = \sum_g \Delta A_g \tag{7.6-9}$$

$$\Delta S = \sum_g \Delta S_g \tag{7.6-10}$$

$$\Delta L = \sum_g \Delta L_g \tag{7.6-11}$$

$$\Delta DB^2 = \sum_g \Delta DB_g^2 \tag{7.6-12}$$

$$\Delta\nu\Sigma_{f\,g}(\boldsymbol{r}) = \nu\Sigma_{f\,g}^{p}(\boldsymbol{r}) - \nu\Sigma_{f\,g}(\boldsymbol{r}) \tag{7.6-13}$$

$$\Delta\chi_g(\boldsymbol{r}) = \chi_g^{p}(\boldsymbol{r}) - \chi_g(\boldsymbol{r}) \tag{7.6-14}$$

$$\Delta\Sigma_{a\,g}(\boldsymbol{r}) = \Sigma^{p}_{a\,g}(\boldsymbol{r}) - \Sigma_{a\,g}(\boldsymbol{r}) \tag{7.6-15}$$

$$\Delta\Sigma_{s\,g\to g'}(\boldsymbol{r}) = \Sigma^{p}_{s\,g\to g'}(\boldsymbol{r}) - \Sigma_{s\,g\to g'}(\boldsymbol{r}) \tag{7.6-16}$$

$$\Delta D_g(\boldsymbol{r}) = D^{p}_g(\boldsymbol{r}) - D_g(\boldsymbol{r}) \tag{7.6-17}$$

$$\Delta B^2_g(\boldsymbol{r}) = B^{2\,p}_g(\boldsymbol{r}) - B^2_g(\boldsymbol{r}) \tag{7.6-18}$$

The superscript *p* denotes the perturbed state.

7.6.2 Finite-difference Equation for Leakage Term

The term appearing in the leakage term $\nabla\varphi^{*}_g(\boldsymbol{r})\Delta D_g(\boldsymbol{r})\nabla\varphi_g(\boldsymbol{r})dV$ is approximated as shown below.

$$\sum_j A_j \frac{1}{\Delta_i}\left\{\frac{\Delta_i D_{jg}}{\Delta_i D_{jg} + \Delta_j D_{ig}}\right\}^2 \left\{\varphi^{*}_{ig} - \varphi^{*}_{jg}\right\}\left\{\varphi_{ig} - \varphi_{jg}\right\} \quad \text{in the bulk of the system}$$

$$\sum_j A_j \frac{1}{\Delta_i}\left\{\frac{\Delta_i C_{sg}}{\Delta_i C_{sg} + \Delta_j D_{ig}}\right\}^2 \varphi^{*}_{ig}\varphi_{ig} \quad \text{at the black boundary of the system}$$

where the subscript *i* denotes a flux point, *j* the neighboring flux point, A_j the leakage area, Δi the distance between the flux point *i* and the leakage surface, Δj the distance between the flux point *j* and the leakage surface, and C_{sg} the black boundary constant. At the reflective boundary the above term is null.

7.7 Cell Burn-up Calculation

In the cell burn-up calculation, two kinds of time-step units are adopted in the SRAC code. One is the burn-up step unit with a relatively broad time interval, and the other is the sub-step unit in each burn-up step. While the burn-up step interval is specified by input, the sub-step interval is determined in the code. At each burn-up step, flux calculation is carried out with a selected code. As a result, one-group collapsed flux distribution and collapsed microscopic cross-sections for burnable nuclides are obtained. The depletion equation for the interval of the *n*-th burn-up step [t_{n-1}, t_n] can be expressed by Eq. (7.7-1), under the assumption that the relative distribution of the microscopic reaction rates for capture, fission and (n,2n) reactions does not change during the time interval of the burn-up step.

$$\frac{dN_i^M(t)}{dt} = \sum_{j\neq i} f_{j\to i}\lambda_j N_i^M(t) + \sum_{k\neq i}\{g_{k\to i}\sigma_{c,k}^M + \gamma_{k\to i}\sigma_{f,k}^M + h_{k\to i}\sigma_{n2n,k}^M\}\varphi^M Fact(t) N_k^M(t) \\ -[\lambda_i + (\sigma_{a,i}^M + \sigma_{n2n,i}^M)\varphi^M Fact(t)]N_i^M(t) \tag{7.7-1}$$

where i, j, k : depleting nuclides

M : depleting zone, which corresponds to the M-Region in the SRAC code.

N : atomic number density

λ, f : decay constant and branching ratio

γ, g, h : yield fraction of each transmutation,

φ : relative flux obtained by eigenvalue calculation

$Fact(t)$: Normalization factor to convert relative flux to absolute one

If we assume the thermal power over the cell under consideration is constant (P) during $[t_{n-1}, t_n]$, the normalization factor $Fact(t)$ for the interval of the m-th sub-step $[t_{m-1}, t_m] \in [t_{n-1}, t_n]$ is given by

$$Fact(t_{m-1} \le t \le t_m) = P(t_{m-1} \le t \le t_m) / \sum_M \sum_i \kappa_i N_i^M(t_{m-1}) \sigma_{f,i}^M V^M \tag{7.7-2}$$

where P : Constant power in $[t_{n-1}, t_n]$ given by input data

κ_i : Energy release per fission of the i-th nuclide

Then, Eq. (7.7-1) can be solved analytically by the method of the DCHAIN code[75] for each sub-step. The method of DCHAIN is based on Bateman's method with a modification for more accurate treatment of cyclic burn-up chain caused by α-decay and so on.

The burn-up chain model and parameters such as decay constants and fission yields are installed in the burn-up libraries equipped in the SRAC system. The decay constants are taken from the "Chart of Nuclides 2004"[76]. The fission yields are based on the second version of the JNDC nuclear data library of fission products[77]. Several burn-up chain models[29] are available to be selected by the purpose of the calculation. The library data of each chain model is written in a file of text format, which helps the understanding of the user. The contents can be easily replaced, if necessary (cf. Sect. 3.3).

7.8 One-Point Kinetics Parameters

The following one-point kinetics parameters can be obtained by CITATION of SRAC.

- Effective delayed neutron fraction

$$\beta_{eff} = \sum_i \beta_{eff,i} = \sum_i \left[\frac{\int \sum_g \phi_g^*(\boldsymbol{r}) \chi_{g,i}^d(\boldsymbol{r}) \sum_{g'} \Sigma_{i.g'}^{BVF}(\boldsymbol{r}) \phi_{g'}(\boldsymbol{r}) dV}{\int \sum_g \phi_g^*(\boldsymbol{r}) \chi_g^t(\boldsymbol{r}) \sum_{g'} \nu\Sigma_{f.g'}(\boldsymbol{r}) \phi_{g'}(\boldsymbol{r}) dV} \right] \tag{7.8-1}$$

- Effective decay constant for the *i*-th family of delayed neutron precursor.

$$\frac{1}{\lambda_{eff,i}} = \frac{\int \sum_g \phi_g^*(\boldsymbol{r}) \chi_{g,i}^d(\boldsymbol{r}) \sum_{g'} \Sigma_{i.g'}^{BVL}(\boldsymbol{r}) \phi_{g'}(\boldsymbol{r}) dV}{\int \sum_g \phi_g^*(\boldsymbol{r}) \chi_{g,i}^d(\boldsymbol{r}) \sum_{g'} \Sigma_{i.g'}^{BVF}(\boldsymbol{r}) \phi_{g'}(\boldsymbol{r}) dV} \tag{7.8-2}$$

- Effective delayed neutron life time

$$l = \frac{\int_k \sum_g \phi_g^*(\boldsymbol{r}) \frac{1}{\upsilon_g(\boldsymbol{r})} \phi(\boldsymbol{r}) dV}{\int \sum_g \phi_g^*(\boldsymbol{r}) \frac{\chi_g^t(\boldsymbol{r})}{k_{eff}} \sum_{g'} \nu\Sigma_{f.g'}(\boldsymbol{r}) \phi_{g'}(\boldsymbol{r}) dV} = k_{eff} \Lambda \tag{7.8-3}$$

where,
$$\Sigma_{i,g}^{BVF} \equiv \sum_m \left(\beta_m^i \nu_{g,m} \sigma_{f,g,m} N_m \right) \tag{7.8-4}$$

$$\Sigma_{i,g}^{BVL} \equiv \sum_m \left(\beta_m^i \nu_{g,m} \sigma_{f,g,m} N_m / \lambda_m^i \right) \tag{7.8-5}$$

$$\Sigma_{\upsilon,g} \equiv \sqrt{\frac{1}{\overline{E}_g(eV)}} \approx \sqrt{\frac{1}{(E_{g,Lower} + E_{g,Upper})/2}} \tag{7.8-6}$$

The averaged neutron velocity for the *g*-th group is given by

$$\upsilon_g(\mathrm{m/sec}) = \sqrt{\frac{2 \times 1.60219E-19}{m_n(kg)}} \frac{1}{\Sigma_{\upsilon,g}} = 13831.68 \times \frac{1}{\Sigma_{\upsilon,g}}$$

The macroscopic cross-sections defined by Eqs.(7.8-4), (7.8-5) and (7.8-6) are stored in the MACRO file for the calculation of the one-point kinetics parameters. Theses cross-sections are collapsed and/or homogenized in the same manner (cf. Sec.7.5) as other usual macroscopic cross-sections ($\Sigma_{a,g}$, $\Sigma_{f,g}$, etc.).

8. Tables on Cross-Section Library

8.1 Symbols to denote nuclide

Table 8.1-1 Chemical symbols (zz-Tag)

Z	Element Name	zz-Tag	Z	Element Name	zz-Tag	Z	Element Name	zz-Tag
1	Hydrogen	H0	35	Bromine	BR	71	Lutetium	LU
1	Deuterium	D0	36	Krypton	KR	72	Hafnium	HF
1	Tritium	T0	37	Rubidium	RB	73	Tantalum	TA
2	Helium	HE	38	Strontium	SR	74	Tungsten	W0
3	Lithium	LI	39	Yttrium	Y0	75	Rhenium	RE
4	Beryllium	BE	40	Zirconium	ZR	76	Osmium	OS
5	Boron	B0	41	Nioblium	NB	77	Iridium	IR
6	Carbon	C0	42	Molybdenum	MO	78	Platinium	PT
7	Nitrogen	N0	43	Technetium	TC	79	Gold	AU
8	Oxygen	O0	44	Ruthenium	RU	80	Mercury	HG
9	Fluorine	F0	45	Rhodium	RH	81	Thallium	TL
10	Neon	NE	46	Palladium	PD	82	Lead	PB
11	Sodium	NA	47	Silver	AG	83	Bismuth	BI
12	Magnesium	MG	48	Cadmium	CD	84	Polonium	PO
13	Aluminium	AL	49	Indium	IN	85	Astatine	AT
14	Silicon	SI	50	Tin	SN	86	Radon	RN
15	Phosphorus	P0	51	Antimony	SB	87	Francium	FR
16	Sulfur	S0	52	Tellurium	TE	88	Radium	RA
17	Chlorine	CL	53	Iodine	I0	89	Actinium	AC
18	Argon	AR	54	Xenon	XE	90	Thorium	TH
19	Potassium	K0	55	Cesium	CS	91	Protactinium	PA
20	Calcium	CA	56	Barium	BA	92	Uranium	U0
21	Scandium	SC	57	Lanthane	LA	93	Neptunium	NP
22	Titanium	TI	58	Cerium	CE	94	Plutonium	PU
23	Vanadium	V0	59	Praseodymium	PR	95	Americium	AM
24	Chromium	CR	60	Neodymium	ND	96	Curium	CM
25	Manganese	MN	61	Promethium	PM	97	Berkelium	BK
26	Iron	FE	62	Samarium	SM	98	Californium	CF
27	Cobalt	CO	63	Europium	EU	99	Einsteinium	ES
28	Nickel	NI	64	Gadolinium	GD	100	Fermium	FM
29	Copper	CU	65	Terbium	TB	101	Mendelevium	MD
30	Zinc	ZN	66	Dysprosium	DY	102	Nobelium	NO
31	Gallium	GA	67	Holmium	HO	103	Lawrencium	LR
32	Germanium	GE	68	Erbium	ER	104	Kurchatovium	KU
33	Arsenic	AS	69	Thulium	TM			
34	Selenium	SE	70	Ytterbium	YB			

Specification of nuclide in the input of SRAC is performed by 8 characters in the form Xzzmc00t, where zz-Tag denotes element by 2 characters of chemical symbol as shown in Table 8.1-1, *m*-Tag the last digit of mass number of nuclide, *c*-Tag one character for chemical binding in Table 8.1-3, and *t*-tag for material temperature in Table 8.1-4.

In principle, the *m*-tag denotes mass number, for example, *m*=5 for U-235. If cross-sections of a stable element of natural isotopes abundance is compiled in the library, *m*-tag=N is given (e.g. FEN for Fe-natural.). Table 8.1-2 shows the list of *zz*-tag and *m*-tag of the nuclides with ambiguity or exceptional treatments.

Table 8.1-2 (1/2) Element index (zzm-Tag) for the nuclides with ambiguity or exceptional treatments

(a) Nuclides with many isotopes

Z=44		Z=48		Z=50		Z=52		Z=54		Z=56		Z=62	
RUG	Ru-96	CDG	Cd-106	SNC	Sn-112	TEA	Te-120	XEE	Xe-124	BAA	Ba-130	SME	Sm-144
RU7	Ru-97	CD7	Cd-107	SNE	Sn-114	TE1	Te-121	XEG	Xe-126	BA1	Ba-131	SM7	Sm-147
RU8	Ru-98	CD8	Cd-108	SN5	Sn-115	TE2	Te-122	XE8	Xe-128	BA2	Ba-132	SM8	Sm-148
RU9	Ru-99	CD9	Cd-109	SN6	Sn-116	TE3	Te-123	XE9	Xe-129	BA3	Ba-133	SM9	Sm-149
RU0	Ru-100	CD0	Cd-110	SN7	Sn-117	TE4	Te-124	XE0	Xe-130	BA4	Ba-134	SM0	Sm-150
RU1	Ru-101	CD1	Cd-111	SN8	Sn-118	TE5	Te-125	XE1	Xe-131	BA5	Ba-135	SM1	Sm-151
RU2	Ru-102	CD2	Cd-112	SN9	Sn-119	TE6	Te-126	XE2	Xe-132	BA6	Ba-136	SM2	Sm-152
RU3	Ru-103	CD3	Cd-113	SN0	Sn-120	TE7	Te-127m	XE3	Xe-133	BA7	Ba-137	SM3	Sm-153
RU4	Ru-104	CD4	Cd-114	SN1	Sn-121	TE8	Te-128	XE4	Xe-134	BA8	Ba-138	SM4	Sm-154
RU5	Ru-105	CD5	Cd-115	SN2	Sn-122	TE9	Te-129m	XE5	Xe-135	BA9	Ba-139		
RU6	Ru-106	CDM	Cd-115m	SN3	Sn-123	TE0	Te-130	XE6	Xe-136	BA0	Ba-140		
		CD6	Cd-116	SN4	Sn-124	TEC	Te-132						
				SNF	Sn-125								
				SNG	Sn-126								

Z=94		Z=96	
PU0	Ru-96	CM0	Cm-240
PU1	Ru-97	CM1	Cm-241
PU2	Ru-98	CM2	Cm-242
PU4	Pu-23	CM3	Cm-243
PU6	Pu-236	CM4	Cm-244
PU7	Pu-237	CM5	Cm-245
PU8	Pu-238	CM6	Cm-246
PU9	Pu-239	CM7	Cm-247
PUG	Pu-246	CM8	Cm-248
RUG	Ru-96	CM9	Cm-249
RU7	Ru-97	CMA	Cm-250
RU8	Ru-98		

(b) Nuclides with meta-stable excited states

AMG	Ground state of Am-242 (Am-242g)
AMM	Excited state of Am-242 (Am-242m)
AMT	Excited state of Am-244 (AM-244m)
PMG	Ground state of Pm-148 (Pm-148g)
PMM	Excited state of Pm-148 (Pm-148m)
TE7	Excited state of Te-127 (Te-127m)
TE9	Excited state of Te-129 (Te-129m)
AG0	Excited state of Ag-110 (Ag-110m)

Table 8.1-2 (2/2) Element index (zzm-Tag) for the nuclides with ambiguity or exceptional treatments

(c) Pseudo fission products for cell burn-up calculation

XZ50	Pseudo FP for the burnup chain models (*fp50bp16*)
XZ99	Pseudo FP for the burnup chain models (*fp104bp12*)
XZ66	Pseudo FP for the old burnup chain model (ucm66fp)[3)]
XZ35	Pseudo FP by U-235 fission used in the old simplified burnup chain model (ucm34fp)[3)]
XZ38	Pseudo FP by U-238 fission used in the old simplified burnup chain model (ucm34fp)
XZ39	Pseudo FP by Pu-239 fission used in the old simplified burnup chain model (ucm34fp)
XZ31	Pseudo FP by Pu-241 fission used in the old simplified burnup chain model (ucm34fp)
XZ32	Pseudo FP by Th-232 fission used in the old simplified burnup chain model (ucm34fp)
XZ33	Pseudo FP by U-233 fission used in the old simplified burnup chain model (ucm34fp)

Table 8.1-3 Chemical bounding symbols (*c*-tag)

Compound	*c*-tag	Chemical symbol	Remarks (combination)
Beryllium metal	B	Be	XBE9B000
Beryllium oxide	E	BeO	XBE9E000+XO06E000
Benzene	Q	C_6H_6	XC02Q000+XH01Q000
Graphite	C	C	XC02C000
Polyethylene	P	$(CH_2)_n$	2(XH01P000)+XC020001(free)
Uranium carbite	V	UC	Not yet compiled
Uranium oxide	W	UO2	XU08W000+2(XO06W000) [not used now]
Light water	H	H2O	2(XH01H000)+XO060000(free)
Heavy water	D	D2O	2(XD02D000)+XO060000(free)
Zirconium hydrate	Z	ZrH	XZRNZ000+XH01Z000 or ZR*m*Z0000+XH01Z000 (*m*: *m*-Tag of natural isotopes of Zr)
Free atom	0(zero)	*	Ex. XU050000, XH010000

Note: Use with pairing nuclide(s) specified by "+" in Remarks column.

Table 8.1-4 Temperature symbols (t-tag)

t-tag	1	2	3	4	5	6	7	8	9	A	B
Temperature(K)	300	325	350	400	450	500	550	600	900	1200	2100

As materials at arbitrary temperatures become available in the current SRAC, temperature tag shown above in the material specification (Sect.2.9) has no more practical meaning. However, the *t*-tag corresponding to the temperature nearest to the material temperature is filled to the eighth character of the member name of the effective microscopic cross-sections written on MICREF file.

8.2 List of Public Libraries

The following nine Public Libraries are available in the SRAC system:

(1) SRACLIB-JDL33

Nuclear data file : JENDL-3.3[9)]

Number of nuclides : 396 (including supplemented nuclides, pseudo FPs, etc.)

Remarks : Data of several nuclides whose cross-sections are not evaluated in JENDL-3.3 are supplemented by those based on other nuclear data files (e.g. Dy isotopes). They are shown in Table 8.2-1).
Thermal scattering data $S(\alpha,\beta)$ is based on ENDF/B-VI.
Data for the nuclide with natural isotopes abundance are composed from the nuclear data of constituent isotopes. (c.f. Fe-nat., Cr-nat., Cu-nat., Ni-nat.)

(2) SRACLIB-JDL32

Nuclear data file : JENDL-3.2[78)]

Number of nuclides : 396 (including supplemented nuclides, pseudo FPs, etc.)

Remarks : Data of several nuclides whose cross-sections are not evaluated in JENDL-3.2 are based on other nuclear data files (e.g. Er isotopes).

(3) SRACLIB-JEF31

Nuclear data file : JEFF-3.1[10)]

Number of nuclides : 412 (including pseudo FPs, etc.)

Remarks : Data for the nuclide with natural isotopes abundance are composed from the nuclear data of constituent isotopes. (c.f. Fe-nat.)
Thermal scattering data $S(\alpha,\beta)$ is based on JEFF-3.1.
Delayed neutron data is replaced by JEF-2.2 data because current SRAC can not treat 8 delayed neutron families.

(4) SRACLIB-JEF30

Nuclear data file : JEFF-3.0[79)]

Number of nuclides : 367 (including supplemented nuclides, pseudo FPs, etc.)

Remarks : Data of several nuclides whose cross-sections are not evaluated in

JEFF-3.0 are based on other nuclear data files (See the help file in the library).

Data for the nuclide with natural isotopes abundance are composed from the nuclear data of constituent isotopes. (c.f. Fe-nat.)

Delayed neutron data is replaced by JEF-2.2 because of inconsistent number of delayed neutron family (6 or 8 mixed among nuclides).

(5) SRACLIB-JEF22

Nuclear data file : JEF-2.2[80)]

Number of nuclides : 326 (including supplemented nuclides, pseudo FPs, etc.)

Remarks : Data of several nuclides whose cross-sections are not evaluated in JEF-2.2 are based on other nuclear data files (See help file in the library).

Thermal scattering data $S(\alpha,\beta)$ is based on ENDF/B-III.

(6) SRACLIB-EDF70

Nuclear data file : ENDF/B-VII.0[11)]

Number of nuclides : about 436 (including pseudo FPs, etc.)

Remarks : Data for the nuclide with natural isotopes abundance are composed from the nuclear data of constituent isotopes. (c.f. Fe-nat.)

Thermal scattering data $S(\alpha,\beta)$ is based on ENDF/B-VII.0.

(7) SRACLIB-EDF68

Nuclear data file : ENDF/B-VI.8[81)]

Number of nuclides : 360 (including supplemented nuclides, pseudo FPs, etc.)

Remarks : Data of several nuclides whose cross-sections are not evaluated in ENDF/B-VI.8 are based on other nuclear data files (See help file in the library).

Data for the nuclide with natural isotopes abundance are composed from the nuclear data of constituent isotopes. (c.f. Fe-nat.)

Thermal scattering data $S(\alpha,\beta)$ is based on ENDF/B-VI.

(8) SRACLIB-EDF65

Nuclear data file : ENDF/B-VI.5[82)]

Number of nuclides : 342 (including supplemented nuclides, pseudo FPs, etc.)

Remarks : Data for the nuclide with natural isotopes abundance are composed from the nuclear data of constituent isotopes. (c.f. Fe-nat.)

(9) SRACLIB-EDFB4

Nuclear data file : ENDF/B-IV[83)]

Number of nuclides : 153 (including pseudo FPs)

Each Library has its own installation conductor with help function: ~SRACLIB-*/@PunchMe (C-shell-script). The user can easily install necessary library by using it. Here, a nuclides-list is shown only for the JENDL-3.3 library. For other libraries, it is written in the help file of each library; ~SRACLIB-*/ tool/help/help3.txt.

The explanation of items in Table 8.2-1 follows.

****

FASTDATA	=NO	No self-shielding factor table for fast group constants
	=YES	Self-shielding factor table for fast group constants
F-TABLE NTEMP	Number of temperature points for self-shielding factor table	
	=0	No table
	=1	1 point (usually 293.15K)
	=4	4 points (usually 293.15K, 800K, 2100K, 4500K)
	Temperatures are described in member Czzm0000 in PFAST	
MCROSS LIBRARY	=0	No MCROSS library data for PEACO
	=1	There is MCROSS library data for PEACO
THERMAL F-TAB.	=NO	No self-shielding factor table for thermal group constants
	=YES	Self-shielding factor table for thermal group constants
NTEMP	Number of temperature points for thermal group constants	
	Temperatures are described in member Czzmc000 in PTHERMAL	
THERMAL KERNEL	=P0	P_0 component of thermal scattering matrix
	=P1	P_1 component of thermal scattering matrix
	=P0-Pn	P_0 through P_n components of thermal scattering matrix
	=NO DATA	No thermal scattering matrix

****

Table 8.2-1 (1/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

No	NUCLIDE	FAST DATA	F-TABLE NTEMP	MCROSS LIBRARY	THERMAL F-TAB	NTEMP	THERMAL KERNEL
1	XAC50000	YES	1	NO	NO	1	P0,P1
2	XAC60000	YES	1	NO	NO	1	P0,P1
3	XAC70000	YES	1	NO	NO	1	P0,P1
4	XAG00000	YES	4	NO	NO	10	P0,P1
5	XAG70000	YES	4	YES	NO	10	P0,P1
6	XAG90000	YES	4	YES	YES	10	P0,P1
7	XAL70000	YES	4	NO	NO	10	P0,P1
8	XAM10000	YES	4	YES	YES	10	P0,P1
9	XAM30000	YES	4	YES	YES	10	P0,P1
10	XAM40000	YES	1	NO	NO	1	P0,P1
11	XAMG0000	YES	4	YES	YES	10	P0,P1
12	XAMM0000	YES	4	YES	YES	10	P0,P1
13	XAMT0000	YES	1	NO	NO	1	P0,P1
14	XAR00000	YES	4	NO	NO	10	P0,P1
15	XAS50000	YES	4	NO	NO	1	NO DATA
16	XAU70000 (b62)	YES	4	YES	YES	10	P0,P1
17	XB000000	YES	1	NO	NO	10	P0,P1
18	XB010000	YES	1	NO	NO	10	P0,P1
19	XBA00000	YES	4	NO	NO	1	NO DATA
20	XBA20000	YES	4	NO	NO	1	NO DATA
21	XBA40000	YES	4	NO	NO	1	NO DATA
22	XBA50000	YES	4	NO	NO	1	NO DATA
23	XBA60000	YES	4	NO	NO	1	NO DATA
24	XBA70000	YES	4	NO	NO	1	NO DATA
25	XBA80000	YES	4	NO	NO	1	NO DATA
26	XBAA0000	YES	4	NO	NO	1	NO DATA
27	XBE90000	YES	1	NO	NO	10	P0,P1
28	XBE9B000	YES	1	NO	NO	8	P0-P3
29	XBE9E000	YES	1	NO	NO	8	P0-P3
30	XBI90000	YES	4	NO	NO	10	P0,P1
31	XBK00000	YES	4	NO	YES	1	P0,P1
32	XBK70000	YES	4	NO	YES	10	P0,P1
33	XBK90000	YES	4	NO	YES	1	P0,P1
34	XBR10000	YES	4	NO	NO	1	NO DATA
35	XBR90000	YES	4	NO	NO	1	NO DATA
36	XC020000	YES	1	NO	NO	10	P0-P3
37	XC02C000	YES	1	NO	NO	10	P0-P3
38	XC02Q000	YES	1	NO	NO	8	NO DATA
39	XCA00000	YES	4	NO	NO	10	P0,P1
40	XCA20000	YES	4	NO	NO	10	P0,P1
41	XCA30000	YES	4	NO	NO	10	P0,P1
42	XCA40000	YES	4	NO	NO	10	P0,P1
43	XCA60000	YES	4	NO	NO	10	P0,P1
44	XCA80000	YES	4	NO	NO	10	P0,P1
45	XCAN0000 (comp)	YES	4	NO	NO	10	P0,P1
46	XCD00000	YES	4	NO	NO	10	P0,P1
47	XCD10000	YES	4	NO	NO	10	P0,P1
48	XCD20000	YES	4	NO	NO	10	P0,P1
49	XCD30000	YES	4	NO	YES	10	P0,P1

Table 8.2-1 (2/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

50	XCD40000	YES	4	NO	NO	10	P0,P1
51	XCD60000	YES	4	NO	NO	10	P0,P1
52	XCD80000	YES	4	NO	NO	10	P0,P1
53	XCDG0000	YES	4	NO	NO	10	P0,P1
54	XCE00000	YES	4	NO	NO	1	NO DATA
55	XCE10000	YES	4	NO	NO	1	NO DATA
56	XCE20000	YES	4	NO	NO	1	NO DATA
57	XCE30000 (b62)	YES	1	NO	NO	1	NO DATA
58	XCE40000	YES	4	NO	NO	1	NO DATA
59	XCF00000	YES	4	NO	YES	1	P0,P1
60	XCF10000	YES	4	NO	YES	1	P0,P1
61	XCF20000	YES	4	NO	YES	1	P0,P1
62	XCF30000 (b62)	YES	4	NO	YES	1	P0,P1
63	XCF40000	YES	1	NO	NO	1	P0,P1
64	XCF90000	YES	4	NO	YES	10	P0,P1
65	XCL50000	YES	4	NO	NO	10	P0,P1
66	XCL70000	YES	4	NO	NO	10	P0,P1
67	XCLN0000 (comp)	YES	4	NO	NO	10	P0,P1
68	XCM00000	YES	4	NO	NO	10	P0,P1
69	XCM10000	YES	4	NO	YES	10	P0,P1
70	XCM20000	YES	4	NO	NO	10	P0,P1
71	XCM30000	YES	4	NO	YES	10	P0,P1
72	XCM40000	YES	4	YES	NO	10	P0,P1
73	XCM50000	YES	4	YES	YES	10	P0,P1
74	XCM60000	YES	4	NO	YES	10	P0,P1
75	XCM70000	YES	4	NO	YES	10	P0,P1
76	XCM80000	YES	4	NO	NO	10	P0,P1
77	XCM90000	YES	4	NO	NO	10	P0,P1
78	XCMA0000	YES	4	NO	YES	10	P0,P1
79	XCO90000	YES	4	NO	NO	10	P0,P1
80	XCR00000	YES	4	NO	NO	10	P0,P1
81	XCR20000	YES	4	NO	NO	10	P0,P1
82	XCR30000	YES	4	NO	NO	10	P0,P1
83	XCR40000	YES	4	NO	NO	10	P0,P1
84	XCRN0000 (comp)	YES	4	NO	NO	10	P0,P1
85	XCS30000	YES	4	YES	NO	1	NO DATA
86	XCS40000	YES	4	NO	NO	1	NO DATA
87	XCS50000	YES	4	NO	NO	1	NO DATA
88	XCS60000	YES	4	NO	NO	1	NO DATA
89	XCS70000	YES	4	NO	NO	10	P0,P1
90	XCU30000	YES	4	NO	NO	10	P0,P1
91	XCU50000	YES	4	NO	NO	10	P0,P1
92	XCUN0000 (comp)	YES	4	NO	NO	10	P0,P1
93	XD020000	NO	0	NO	NO	10	P0-P3
94	XD02D000	NO	0	NO	NO	8	P0-P3
95	XDY00000 (b67)	YES	4	NO	NO	1	NO DATA
96	XDY10000 (b67)	YES	4	NO	NO	1	NO DATA
97	XDY20000 (b67)	YES	4	NO	NO	1	NO DATA
98	XDY30000 (b67)	YES	4	NO	NO	1	NO DATA
99	XDY40000 (b67)	YES	4	NO	NO	1	NO DATA
100	XER00000	YES	4	YES	NO	10	P0,P1
101	XER20000	YES	4	NO	NO	10	P0,P1

Table 8.2-1 (3/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

102	XER40000	YES	4	YES	NO	10	P0,P1
103	XER60000	YES	4	YES	NO	10	P0,P1
104	XER70000	YES	4	YES	YES	10	P0,P1
105	XER80000	YES	4	YES	NO	10	P0,P1
106	XES30000 (b62)	YES	4	NO	YES	1	P0,P1
107	XES40000	YES	1	NO	NO	1	P0,P1
108	XES50000	YES	1	NO	NO	1	P0,P1
109	XEU10000	YES	4	NO	YES	10	P0,P1
110	XEU20000	YES	4	NO	YES	10	P0,P1
111	XEU30000	YES	4	NO	YES	10	P0,P1
112	XEU40000	YES	4	NO	YES	10	P0,P1
113	XEU50000	YES	4	NO	YES	10	P0,P1
114	XEU60000	YES	4	NO	YES	10	P0,P1
115	XEU70000 (b62)	YES	1	NO	NO	1	NO DATA
116	XF090000	YES	4	NO	NO	10	P0-P3
117	XFE40000	YES	4	NO	NO	10	P0,P1
118	XFE60000	YES	4	NO	NO	10	P0,P1
119	XFE70000	YES	4	NO	NO	10	P0,P1
120	XFE80000	YES	4	NO	NO	10	P0,P1
121	XFEN0000 (comp)	YES	4	NO	NO	10	P0,P1
122	XFM50000	YES	1	NO	NO	1	P0,P1
123	XGA10000	YES	4	NO	NO	10	P0,P1
124	XGA90000	YES	4	NO	NO	10	P0,P1
125	XGD00000	YES	4	YES	NO	10	P0,P1
126	XGD20000	YES	4	NO	YES	10	P0,P1
127	XGD40000	YES	4	NO	NO	10	P0,P1
128	XGD50000	YES	4	YES	YES	10	P0,P1
129	XGD60000	YES	4	YES	NO	10	P0,P1
130	XGD70000	YES	4	YES	YES	10	P0,P1
131	XGD80000	YES	4	YES	NO	10	P0,P1
132	XGE00000	YES	4	NO	NO	10	P0,P1
133	XGE20000	YES	4	NO	NO	10	P0,P1
134	XGE30000	YES	4	NO	NO	10	P0,P1
135	XGE40000	YES	4	NO	NO	10	P0,P1
136	XGE60000	YES	4	NO	NO	10	P0,P1
137	XGEN0000 (comp)	YES	4	NO	NO	10	P0,P1
138	XH010000	NO	0	NO	NO	10	P0-P3
139	XH01H000	NO	0	NO	NO	8	P0-P5
140	XH01P000	NO	0	NO	NO	2	P0-P3
141	XH01Q000	NO	0	NO	NO	8	P0-P3
142	XH01Z000	NO	0	NO	NO	8	P0-P3
143	XHE30000	YES	1	NO	NO	10	P0,P1
144	XHE40000	YES	1	NO	NO	10	P0,P1
145	XHF00000	YES	4	YES	NO	10	P0,P1
146	XHF40000	YES	4	YES	NO	10	P0,P1
147	XHF60000	YES	4	NO	NO	10	P0,P1
148	XHF70000	YES	4	YES	YES	10	P0,P1
149	XHF80000	YES	4	YES	NO	10	P0,P1
150	XHF90000	YES	4	YES	NO	10	P0,P1
151	XHG00000	YES	4	NO	NO	10	P0,P1
152	XHG10000	YES	4	YES	NO	10	P0,P1
153	XHG20000	YES	4	NO	NO	10	P0,P1

Table 8.2-1 (4/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

154	XHG40000	YES	4	NO	NO	10	P0,P1
155	XHG60000	YES	4	NO	NO	10	P0,P1
156	XHG80000	YES	4	YES	NO	10	P0,P1
157	XHG90000	YES	4	YES	NO	10	P0,P1
158	XHO50000 (b65)	YES	4	NO	YES	10	P0,P1
159	XI000000 (b62)	YES	1	NO	NO	1	NO DATA
160	XI010000	YES	4	NO	NO	1	NO DATA
161	XI050000 (b62)	YES	1	NO	NO	1	NO DATA
162	XI070000	YES	4	NO	NO	1	NO DATA
163	XI090000	YES	4	NO	NO	1	NO DATA
164	XIN30000	YES	4	YES	YES	10	P0,P1
165	XIN50000	YES	4	YES	YES	10	P0,P1
166	XK000000	YES	4	NO	NO	10	P0,P1
167	XK010000	YES	4	NO	NO	10	P0,P1
168	XK090000	YES	4	NO	NO	10	P0,P1
169	XK0N0000 (comp)	YES	4	NO	NO	10	P0,P1
170	XKR00000	YES	4	NO	NO	1	NO DATA
171	XKR20000	YES	4	NO	NO	1	NO DATA
172	XKR30000	YES	4	NO	NO	1	NO DATA
173	XKR40000	YES	4	NO	NO	1	NO DATA
174	XKR50000	YES	4	NO	NO	1	NO DATA
175	XKR60000	YES	4	NO	NO	1	NO DATA
176	XKR80000	YES	4	NO	NO	1	NO DATA
177	XLA00000 (b62)	YES	1	NO	NO	1	NO DATA
178	XLA80000	YES	4	NO	NO	1	NO DATA
179	XLA90000	YES	4	NO	NO	1	NO DATA
180	XLI60000	YES	1	NO	NO	10	P0,P1
181	XLI70000	YES	1	NO	NO	10	P0,P1
182	XMG40000	YES	4	NO	NO	10	P0,P1
183	XMG50000	YES	4	NO	NO	10	P0,P1
184	XMG60000	YES	4	NO	NO	10	P0,P1
185	XMGN0000 (comp)	YES	4	NO	NO	10	P0,P1
186	XMN50000	YES	4	NO	NO	10	P0,P1
187	XMO00000	YES	4	NO	NO	10	P0,P1
188	XMO20000	YES	4	NO	NO	10	P0,P1
189	XMO40000	YES	4	NO	NO	10	P0,P1
190	XMO50000	YES	4	NO	NO	10	P0,P1
191	XMO60000	YES	4	NO	NO	10	P0,P1
192	XMO70000	YES	4	NO	NO	10	P0,P1
193	XMO80000	YES	4	NO	NO	10	P0,P1
194	XMO90000	YES	4	NO	NO	1	NO DATA
195	XMON0000 (comp)	YES	4	NO	NO	10	P0,P1
196	XN040000	YES	1	NO	NO	10	P0-P3
197	XN050000	YES	1	NO	NO	10	P0-P3
198	XNA30000	YES	4	NO	NO	10	P0,P1
199	XNB30000	YES	4	NO	NO	10	P0,P1
200	XNB40000	YES	4	NO	NO	1	NO DATA
201	XNB50000	YES	4	NO	NO	1	NO DATA
202	XND00000	YES	4	NO	NO	1	NO DATA
203	XND20000	YES	4	NO	NO	1	NO DATA
204	XND30000	YES	4	NO	NO	1	NO DATA
205	XND40000	YES	4	NO	NO	1	NO DATA

Table 8.2-1 (5/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

206	XND50000	YES	4	NO	NO	1	NO DATA
207	XND60000	YES	4	NO	NO	1	NO DATA
208	XND70000	YES	4	NO	NO	1	NO DATA
209	XND80000	YES	4	NO	NO	1	NO DATA
210	XNI00000	YES	4	NO	NO	10	P0,P1
211	XNI10000	YES	4	NO	NO	10	P0,P1
212	XNI20000	YES	4	NO	NO	10	P0,P1
213	XNI40000	YES	4	NO	NO	10	P0,P1
214	XNI80000	YES	4	NO	NO	10	P0,P1
215	XNIN0000 (comp)	YES	4	NO	NO	10	P0,P1
216	XNP50000	YES	1	NO	NO	10	P0,P1
217	XNP60000	YES	1	NO	NO	1	P0,P1
218	XNP70000	YES	4	YES	YES	10	P0,P1
219	XNP80000	YES	1	NO	NO	1	P0,P1
220	XNP90000	YES	1	YES	NO	1	P0,P1
221	XO060000	YES	1	NO	NO	10	P0-P3
222	XO06E000	YES	1	NO	NO	8	NO DATA
223	XP010000	YES	4	NO	NO	10	P0,P1
224	XPA10000	YES	4	NO	YES	10	P0,P1
225	XPA20000	YES	1	NO	NO	1	P0,P1
226	XPA30000	YES	4	NO	YES	10	P0,P1
227	XPB40000	YES	4	NO	NO	10	P0,P1
228	XPB60000	YES	4	NO	NO	10	P0,P1
229	XPB70000	YES	4	NO	NO	10	P0,P1
230	XPB80000	YES	4	NO	NO	10	P0,P1
231	XPBN0000 (comp)	YES	4	NO	NO	10	P0,P1
232	XPD00000	YES	4	NO	NO	1	NO DATA
233	XPD20000	YES	4	NO	NO	1	NO DATA
234	XPD40000	YES	4	NO	NO	1	NO DATA
235	XPD50000	YES	4	YES	NO	1	NO DATA
236	XPD60000	YES	4	NO	NO	1	NO DATA
237	XPD70000	YES	4	NO	NO	1	NO DATA
238	XPD80000	YES	4	NO	YES	10	P0,P1
239	XPM10000 (b62)	YES	1	NO	NO	1	NO DATA
240	XPM70000	YES	4	NO	NO	1	NO DATA
241	XPM90000	YES	4	NO	YES	10	P0,P1
242	XPMG0000	YES	4	NO	YES	10	P0,P1
243	XPMM0000	YES	4	NO	YES	10	P0,P1
244	XPR10000	YES	4	NO	NO	1	NO DATA
245	XPR30000	YES	4	NO	NO	1	NO DATA
246	XPU00000	YES	4	YES	YES	10	P0,P1
247	XPU10000	YES	4	YES	YES	10	P0,P1
248	XPU20000	YES	4	YES	YES	10	P0,P1
249	XPU40000	YES	4	NO	YES	10	P0,P1
250	XPU60000	YES	4	YES	YES	10	P0,P1
251	XPU70000	YES	1	NO	NO	10	P0,P1
252	XPU80000	YES	4	YES	YES	10	P0,P1
253	XPU90000	YES	4	YES	YES	10	P0,P1
254	XPUG0000	YES	1	NO	NO	1	P0,P1
255	XRA30000	YES	1	NO	NO	1	P0,P1
256	XRA40000	YES	1	NO	NO	1	P0,P1
257	XRA50000	YES	1	NO	NO	1	P0,P1

Table 8.2-1 (6/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

258	XRA60000	YES	4	NO	YES	1	P0,P1
259	XRB50000	YES	4	NO	NO	1	NO DATA
260	XRB60000 (b62)	YES	1	NO	NO	1	NO DATA
261	XRB70000	YES	4	NO	NO	1	NO DATA
262	XRH30000	YES	4	YES	YES	10	P0,P1
263	XRH50000	YES	4	NO	YES	10	P0,P1
264	XRU00000	YES	4	NO	NO	1	NO DATA
265	XRU10000	YES	4	YES	NO	1	NO DATA
266	XRU20000	YES	4	NO	NO	1	NO DATA
267	XRU30000	YES	4	NO	NO	1	NO DATA
268	XRU40000	YES	4	NO	NO	1	NO DATA
269	XRU50000 (b62)	YES	1	NO	NO	1	NO DATA
270	XRU60000	YES	4	NO	NO	1	NO DATA
271	XRU80000	YES	4	NO	NO	1	NO DATA
272	XRU90000	YES	4	NO	NO	1	NO DATA
273	XRUG0000	YES	4	NO	NO	1	NO DATA
274	XS020000	YES	4	NO	NO	10	P0,P1
275	XS030000	YES	4	NO	NO	10	P0,P1
276	XS040000	YES	4	NO	NO	10	P0,P1
277	XS060000	YES	4	NO	NO	10	P0,P1
278	XS0N0000 (comp)	YES	4	NO	NO	10	P0,P1
279	XSB10000	YES	4	NO	NO	10	P0,P1
280	XSB30000	YES	4	NO	NO	10	P0,P1
281	XSB40000	YES	4	NO	YES	10	P0,P1
282	XSB50000	YES	4	NO	NO	1	NO DATA
283	XSB60000 (b62)	YES	1	NO	NO	1	NO DATA
284	XSC50000	YES	4	NO	NO	10	P0,P1
285	XSE00000	YES	4	NO	NO	1	NO DATA
286	XSE20000	YES	4	NO	NO	1	NO DATA
287	XSE40000	YES	4	NO	NO	1	NO DATA
288	XSE60000	YES	4	NO	NO	1	NO DATA
289	XSE70000	YES	4	NO	NO	1	NO DATA
290	XSE80000	YES	4	NO	NO	1	NO DATA
291	XSE90000	YES	4	NO	NO	1	NO DATA
292	XSI00000	YES	4	NO	NO	10	P0,P1
293	XSI80000	YES	4	NO	NO	10	P0,P1
294	XSI90000	YES	4	NO	NO	10	P0,P1
295	XSIN0000 (comp)	YES	4	NO	NO	10	P0,P1
296	XSM00000	YES	4	YES	NO	1	NO DATA
297	XSM10000	YES	4	YES	YES	10	P0,P1
298	XSM20000	YES	4	YES	NO	1	NO DATA
299	XSM30000	YES	4	NO	NO	1	NO DATA
300	XSM40000	YES	4	NO	NO	1	NO DATA
301	XSM70000	YES	4	NO	YES	10	P0,P1
302	XSM80000	YES	4	NO	NO	1	NO DATA
303	XSM90000	YES	4	NO	YES	10	P0,P1
304	XSME0000	YES	4	NO	NO	1	NO DATA
305	XSN00000	YES	4	NO	NO	1	NO DATA
306	XSN20000	YES	4	NO	NO	1	NO DATA
307	XSN30000	YES	4	NO	NO	1	NO DATA
308	XSN40000	YES	4	NO	NO	1	NO DATA
309	XSN50000	YES	4	NO	NO	1	NO DATA

Table 8.2-1 (7/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

310	XSN60000	YES	4	NO	NO	1	NO DATA
311	XSN70000	YES	4	NO	NO	1	NO DATA
312	XSN80000	YES	4	NO	NO	1	NO DATA
313	XSN90000	YES	4	NO	NO	1	NO DATA
314	XSNC0000	YES	4	NO	NO	1	NO DATA
315	XSNE0000	YES	4	NO	NO	1	NO DATA
316	XSNG0000	YES	4	NO	NO	1	NO DATA
317	XSNN0000 (comp)	YES	4	NO	NO	10	P0,P1
318	XSR00000	YES	4	NO	NO	1	NO DATA
319	XSR40000 (b62)	YES	4	NO	NO	1	NO DATA
320	XSR60000	YES	4	NO	NO	1	NO DATA
321	XSR70000	YES	4	NO	NO	1	NO DATA
322	XSR80000	YES	4	NO	NO	1	NO DATA
323	XSR90000	YES	4	NO	NO	1	NO DATA
324	XTA10000	YES	4	YES	YES	10	P0,P1
325	XTB00000 (b62)	YES	1	NO	NO	1	NO DATA
326	XTB90000	YES	4	NO	YES	10	P0,P1
327	XTC90000	YES	4	YES	YES	10	P0,P1
328	XTE00000	YES	4	NO	NO	1	NO DATA
329	XTE20000	YES	4	NO	NO	1	NO DATA
330	XTE30000	YES	4	NO	NO	1	NO DATA
331	XTE40000	YES	4	NO	NO	1	NO DATA
332	XTE50000	YES	4	NO	NO	1	NO DATA
333	XTE60000	YES	4	NO	NO	1	NO DATA
334	XTE70000	YES	4	NO	NO	1	NO DATA
335	XTE80000	YES	4	NO	NO	1	NO DATA
336	XTE90000	YES	4	NO	NO	1	NO DATA
337	XTEA0000	YES	4	NO	NO	1	NO DATA
338	XTEC0000 (b62)	YES	1	NO	NO	1	NO DATA
339	XTH00000	YES	4	NO	YES	1	P0,P1
340	XTH20000	YES	4	YES	NO	10	P0,P1
341	XTH30000	YES	1	NO	NO	1	P0,P1
342	XTH40000	YES	1	NO	NO	1	P0,P1
343	XTH70000	YES	1	NO	NO	1	P0,P1
344	XTH80000	YES	4	NO	YES	1	P0,P1
345	XTH90000	YES	4	NO	YES	1	P0,P1
346	XTI00000	YES	4	NO	NO	10	P0,P1
347	XTI60000	YES	4	NO	NO	10	P0,P1
348	XTI70000	YES	4	NO	NO	10	P0,P1
349	XTI80000	YES	4	NO	NO	10	P0,P1
350	XTI90000	YES	4	NO	NO	10	P0,P1
351	XTIN0000 (comp)	YES	4	NO	NO	10	P0,P1
352	XU020000	YES	4	NO	NO	1	P0,P1
353	XU030000	YES	4	YES	YES	10	P0,P1
354	XU040000	YES	4	YES	NO	10	P0,P1
355	XU050000	YES	4	YES	YES	10	P0,P1
356	XU060000	YES	4	YES	NO	10	P0,P1
357	XU070000	YES	4	NO	YES	10	P0,P1
358	XU080000	YES	4	YES	NO	10	P0,P1
359	XV0N0000	YES	4	NO	NO	10	P0,P1
360	XW020000	YES	4	YES	YES	10	P0,P1
361	XW030000	YES	4	YES	NO	10	P0,P1

Table 8.2-1 (8/8) List of SRAC public library based on JENDL-3.3 (SRACLIB-J33)

362	XW040000	YES	4	YES	NO	10	P0,P1
363	XW060000	YES	4	YES	NO	10	P0,P1
364	XXE00000	YES	4	NO	NO	1	NO DATA
365	XXE10000	YES	4	YES	NO	1	NO DATA
366	XXE20000	YES	4	NO	NO	1	NO DATA
367	XXE30000	YES	4	NO	NO	1	NO DATA
368	XXE40000	YES	4	NO	NO	1	NO DATA
369	XXE50000	YES	4	NO	YES	10	P0,P1
370	XXE60000	YES	4	NO	NO	1	NO DATA
371	XXE80000	YES	4	NO	NO	1	NO DATA
372	XXE90000	YES	4	NO	NO	1	NO DATA
373	XXEE0000	YES	4	NO	NO	1	NO DATA
374	XXEG0000	YES	4	NO	NO	1	NO DATA
375	XY000000 (b62)	YES	1	NO	NO	1	NO DATA
376	XY010000	YES	4	NO	NO	1	NO DATA
377	XY090000	YES	4	NO	NO	1	NO DATA
378	XZ310000 (psd*)	NO	0	NO	NO	1	NO DATA
379	XZ320000 (psd*)	NO	0	NO	NO	1	NO DATA
380	XZ330000 (psd*)	NO	0	NO	NO	1	NO DATA
381	XZ350000 (psd*)	NO	0	NO	NO	1	NO DATA
382	XZ380000 (psd*)	NO	0	NO	NO	1	NO DATA
383	XZ390000 (psd*)	NO	0	NO	NO	1	NO DATA
384	XZ500000 (psd)	NO	0	NO	NO	1	NO DATA
385	XZ660000 (psd*)	NO	0	NO	NO	1	NO DATA
386	XZ990000 (psd)	NO	0	NO	NO	1	NO DATA
387	XZR00000	YES	4	NO	NO	10	P0,P1
388	XZR10000	YES	4	NO	NO	10	P0,P1
389	XZR20000	YES	4	NO	NO	10	P0,P1
390	XZR30000	YES	4	NO	NO	10	P0,P1
391	XZR40000	YES	4	NO	NO	10	P0,P1
392	XZR50000	YES	4	NO	NO	10	P0,P1
393	XZR60000	YES	4	NO	NO	10	P0,P1
394	XZRN0000 (comp)	YES	4	NO	NO	10	P0,P1
395	XZRNZ000	YES	4	NO	NO	8	P0-P3
396	XZRY0000 (b4)	YES	4	NO	NO	10	P0,P1

Note: Some nuclides are supplemented with other nuclear data files
b4 : Based on ENDF/B-IV (no evaluation in JENDL-3.3)
b6# : Based on ENDF/B-VI.# (no evaluation in JENDL-3.3)
----- Natural nuclides
comp : Natural nuclide composed from individual isotope evaluation
----- Special nuclides
psd : Pseudo Fission Products based on JENDL-3.3 for burn-up calculation
psd* : Pseudo Fission Products based on JENDL-3.2

8.3 Energy Group Structure

The energy group structure of the Public Libraries consists of 107 groups: 74 groups for fast and 48 for thermal groups, with 12 overlapping groups. They are shown in Table 8.3-1 and Table 8.3-2, respectively. The user can select a thermal-cut-off energy within the overlapping groups, by taking into account of continuity of cross-sections (cf. Sect.1.3), thermal up-scattering and resonance levels in thermal energy range. The cross-sections of the 107 group structure can be collapsed into the cross-sections of user's fine energy group structure by an asymptotic spectrum (cf. Sect.1.5).

Table 8.3-1 (1/2) Energy group structure of Public Fast Library

Group	Energy (eV)		Velocity (m/s)	Lethargy		Remarks
	Upper	Lower	Upper	Upper	Width	
1	1.00000E+07	7.78800E+06	4.37400E+07	0.0000	0.2500	(1)Fast-Fiss
2	7.78800E+06	6.06530E+06	3.86000E+07	0.2500	0.2500	
3	6.06530E+06	4.72370E+06	3.40640E+07	0.5000	0.2500	
4	4.72370E+06	3.67880E+06	3.00620E+07	0.7500	0.2500	
5	3.67880E+06	2.86510E+06	2.65290E+07	1.0000	0.2500	
6	2.86510E+06	2.23130E+06	2.34120E+07	1.2500	0.2500	
7	2.23130E+06	1.73770E+06	2.06610E+07	1.5000	0.2500	
8	1.73770E+06	1.35340E+06	1.82330E+07	1.7500	0.2500	
9	1.35340E+06	1.05400E+06	1.60910E+07	2.0000	0.2500	
10	1.05400E+06	8.20850E+05	1.42000E+07	2.2500	0.2500	
11	8.20850E+05	6.39280E+05	1.25320E+07	2.5000	0.2500	(2)Smooth
12	6.39280E+05	4.97870E+05	1.10590E+07	2.7500	0.2500	
13	4.97870E+05	3.87740E+05	9.75960E+06	3.0000	0.2500	
14	3.87740E+05	3.01970E+05	8.61280E+06	3.2500	0.2500	
15	3.01970E+05	2.35180E+05	7.60080E+06	3.5000	0.2500	
16	2.35180E+05	1.83160E+05	6.70770E+06	3.7500	0.2500	
17	1.83160E+05	1.42640E+05	5.91950E+06	4.0000	0.2500	
18	1.42640E+05	1.11090E+05	5.22390E+06	4.2500	0.2500	
19	1.11090E+05	8.65170E+04	4.61010E+06	4.5000	0.2500	
20	8.65170E+04	6.73800E+04	4.06840E+06	4.7500	0.2500	
21	6.73800E+04	5.24750E+04	3.59040E+06	5.0000	0.2500	(3)Reson-I
22	5.24750E+04	4.08680E+04	3.16850E+06	5.2500	0.2500	
23	4.08680E+04	3.18280E+04	2.79620E+06	5.5000	0.2500	
24	3.18280E+04	2.47880E+04	2.46760E+06	5.7500	0.2500	
25	2.47880E+04	1.93050E+04	2.17770E+06	6.0000	0.2500	
26	1.93050E+04	1.50340E+04	1.92180E+06	6.2500	0.2500	
27	1.50340E+04	1.17090E+04	1.69600E+06	6.5000	0.2500	
28	1.17090E+04	9.11880E+03	1.49670E+06	6.7500	0.2500	
29	9.11880E+03	7.10170E+03	1.32080E+06	7.0000	0.2500	
30	7.10170E+03	5.53080E+03	1.16560E+06	7.2500	0.2500	
31	5.53080E+03	4.30740E+03	1.02870E+06	7.5000	0.2500	

Table 8.3-1 (2/2) Energy group structure of Public Fast Library

32	4.30740E+03	3.35460E+03	9.07790E+05	7.7500	0.2500	
33	3.35460E+03	2.61260E+03	8.01120E+05	8.0000	0.2500	
34	2.61260E+03	2.03470E+03	7.06990E+05	8.2500	0.2500	
35	2.03470E+03	1.58460E+03	6.23910E+05	8.5000	0.2500	
36	1.58460E+03	1.23410E+03	5.50600E+05	8.7500	0.2500	
37	1.23410E+03	9.61120E+02	4.85900E+05	9.0000	0.2500	
38	9.61120E+02	7.48520E+02	4.28810E+05	9.2500	0.2500	(4) PEACO
39	7.48520E+02	5.82950E+02	3.78420E+05	9.5000	0.2500	
40	5.82950E+02	4.54000E+02	3.33960E+05	9.7500	0.2500	
41	4.54000E+02	3.53580E+02	2.94720E+05	10.0000	0.2500	
42	3.53580E+02	2.75360E+02	2.60090E+05	10.2500	0.2500	
43	2.75360E+02	2.14450E+02	2.29520E+05	10.5000	0.2500	
44	2.14450E+02	1.67020E+02	2.02550E+05	10.7500	0.2500	
45	1.67020E+02	1.30070E+02	1.78750E+05	11.0000	0.2500	
46	1.30070E+02	1.01300E+02	1.57750E+05	11.2500	0.2500	(5)Reso-II
47	1.01300E+02	7.88930E+01	1.39210E+05	11.5000	0.2500	
48	7.88930E+01	6.14420E+01	1.22860E+05	11.7500	0.2500	
49	6.14420E+01	4.78510E+01	1.08420E+05	12.0000	0.2500	
50	4.78510E+01	3.72660E+01	9.56800E+04	12.2500	0.2500	
51	3.72660E+01	2.90230E+01	8.44370E+04	12.5000	0.2500	
52	2.90230E+01	2.26030E+01	7.45160E+04	12.7500	0.2500	
53	2.26030E+01	1.76040E+01	6.57600E+04	13.0000	0.2500	
54	1.76040E+01	1.37100E+01	5.80330E+04	13.2500	0.2500	
55	1.37100E+01	1.06770E+01	5.12140E+04	13.5000	0.2500	
56	1.06770E+01	8.31530E+00	4.51960E+04	13.7500	0.2500	
57	8.31530E+00	6.47590E+00	3.98850E+04	14.0000	0.2500	
58	6.47590E+00	5.04350E+00	3.51990E+04	14.2500	0.2500	
59	5.04350E+00	3.92790E+00	3.10630E+04	14.5000	0.2500	
60	3.92790E+00	3.05900E+00	2.74130E+04	14.7500	0.2500	(6)Overlap
61	3.05900E+00	2.38240E+00	2.41920E+04	15.0000	0.2500	
62	2.38240E+00	1.85540E+00	2.13490E+04	15.2500	0.2500	
63	1.85540E+00	1.63740E+00	1.88410E+04	15.5000	0.1250	
64	1.63740E+00	1.44500E+00	1.76990E+04	15.6250	0.1250	
65	1.44500E+00	1.27520E+00	1.66270E+04	15.7500	0.1250	
66	1.27520E+00	1.12540E+00	1.56190E+04	15.8750	0.1250	
67	1.12540E+00	9.93120E-01	1.46730E+04	16.0000	0.1250	
68	9.93120E-01	8.76430E-01	1.37840E+04	16.1250	0.1250	
69	8.76430E-01	7.73440E-01	1.29490E+04	16.2500	0.1250	
70	7.73440E-01	6.82560E-01	1.21640E+04	16.3750	0.1250	
71	6.82560E-01	6.02360E-01	1.14270E+04	16.5000	0.1250	
72	6.02360E-01	5.31580E-01	1.07350E+04	16.6250	0.1250	
73	5.31580E-01	4.69120E-01	1.00850E+04	16.7500	0.1250	
74	4.69120E-01	4.13990E-01	9.47360E+03	16.8750	0.1250	

(1) Upper Boundary of Fast Fission Range

(2) Upper Boundary of Smooth Range

(3) Upper Boundary of Resonance-I Range

(4) Upper Boundary of PEACO Routine, depending on Input IC8 in Sect.2.2

(5) Upper Boundary of Resonance-II Range, IR Approximation(if IC5=1 in Sect.2.2)

(6) Upper Energy Overlapping with Thermal Energy Range (1.85540 eV is recommended for water moderated system)

Table 8.3-2 (1/2) Energy group structure of Public Thermal Library

Group	Energy (eV)		Velocity (m/s)	Lethargy		Remarks
	Upper	Lower	Upper	Upper	Width	
1	3.92790E+00	3.05900E+00	2.74130E+04	14.7500	0.2500	
2	3.05900E+00	2.38240E+00	2.41920E+04	15.0000	0.2500	
3	2.38240E+00	1.85540E+00	2.13490E+04	15.2500	0.2500	
4	1.85540E+00	1.63740E+00	1.88410E+04	15.5000	0.1250	
5	1.63740E+00	1.44500E+00	1.76990E+04	15.6250	0.1250	
6	1.44500E+00	1.27520E+00	1.66270E+04	15.7500	0.1250	
7	1.27520E+00	1.12540E+00	1.56190E+04	15.8750	0.1250	
8	1.12540E+00	9.93120E-01	1.46730E+04	16.0000	0.1250	
9	9.93120E-01	8.76420E-01	1.37840E+04	16.1250	0.1250	
10	8.76420E-01	7.73440E-01	1.29490E+04	16.2500	0.1250	
11	7.73440E-01	6.82560E-01	1.21640E+04	16.3750	0.1250	
12	6.82560E-01	6.02360E-01	1.14270E+04	16.5000	0.1250	
13	6.02360E-01	5.31580E-01	1.07350E+04	16.6250	0.1250	
14	5.31580E-01	4.69120E-01	1.00850E+04	16.7500	0.1250	
15	4.69120E-01	4.13990E-01	9.47360E+03	16.8750	0.1250	(1)Overlap
16	4.13990E-01	3.89260E-01	8.89960E+03	17.0000	0.0616	$\Delta\upsilon$ =270m/s
17	3.89260E-01	3.65280E-01	8.62970E+03	17.0616	0.0636	:
18	3.65280E-01	3.42060E-01	8.35960E+03	17.1252	0.0657	:
19	3.42060E-01	3.19610E-01	8.08960E+03	17.1909	0.0679	:
20	3.19610E-01	2.97920E-01	7.81960E+03	17.2587	0.0703	:
21	2.97920E-01	2.76990E-01	7.54960E+03	17.3290	0.0728	:
22	2.76990E-01	2.56830E-01	7.27960E+03	17.4019	0.0756	:
23	2.56830E-01	2.37420E-01	7.00970E+03	17.4774	0.0786	:
24	2.37420E-01	2.18780E-01	6.73960E+03	17.5560	0.0818	:
25	2.18780E-01	2.00900E-01	6.46960E+03	17.6378	0.0853	:
26	2.00900E-01	1.83780E-01	6.19960E+03	17.7230	0.0891	:
27	1.83780E-01	1.67430E-01	5.92960E+03	17.8121	0.0932	:
28	1.67430E-01	1.51830E-01	5.65970E+03	17.9053	0.0978	:
29	1.51830E-01	1.37000E-01	5.38960E+03	18.0031	0.1028	:
30	1.37000E-01	1.22930E-01	5.11960E+03	18.1059	0.1084	:
31	1.22930E-01	1.09630E-01	4.84960E+03	18.2142	0.1145	:
32	1.09630E-01	9.70800E-02	4.57970E+03	18.3287	0.1216	:
33	9.70800E-02	8.53970E-02	4.30960E+03	18.4503	0.1282	:
34	8.52970E-02	7.42760E-02	4.04200E+03	18.5785	0.1395	:
35	7.42760E-02	6.40170E-02	3.76960E+03	18.7181	0.1486	:
36	6.40170E-02	5.45200E-02	3.49960E+03	18.8667	0.1606	:
37	5.45200E-02	4.57850E-02	3.22960E+03	19.0273	0.1746	:

Table 8.3-2 (2/2) Energy group structure of Public Thermal Library

38	4.57850E-02	3.78130E-02	2.95960E+03	19.2019	0.1913	:
39	3.78130E-02	3.06020E-02	2.68960E+03	19.3932	0.2116	:
40	3.06020E-02	2.41540E-02	2.41960E+03	19.6048	0.2366	:
41	2.41540E-02	1.84670E-02	2.14970E+03	19.8414	0.2685	:
42	1.84670E-02	1.35430E-02	1.87960E+03	20.1099	0.3101	:
43	1.35430E-02	9.38050E-03	1.60970E+03	20.4200	0.3672	:
44	9.38050E-03	5.98040E-03	1.33960E+03	20.7872	0.4501	:
45	5.98040E-03	3.34230E-03	1.06960E+03	21.2374	0.5818	:
46	3.34230E-03	1.46630E-03	7.99650E+02	21.8192	0.8239	:
47	1.46630E-03	3.52380E-04	5.29650E+02	22.6431	1.4258	:
48	3.52380E-04	1.00000E-05	2.59650E+02	24.0689	3.5621	:
48L	1.00000E-05	**********	4.37380E+01	27.6310	******	

(1) Lower Energy Overlapping with Fast Energy Range

References

1) K. Tsuchihashi, H. Takano, K. Horikami, Y. Ishiguro, K. Kaneko and T. Hara: “SRAC: JAERI Thermal Reactor Standard Code System for Reactor Design and Alalysis,” JAERI 1285 (1983).
2) K. Tsuchihashi, Y. Ishiguro, K. Kaneko and M. Ido: “Revised SRAC Code System,” JAERI 1302 (1986).
3) K. Okumura, K. Kaneko, and K. Tsuchihashi, “SRAC95; General Purpose Neutronics Code System,” JAERI-Data/Code 96-015 (1996), [in Japanese].
4) W. W. Engle Jr: “A User’s Manual for ANISN,” K-1693 (1967).
5) K. D. Lathlop and F. W. Brinkly: “Theory and Use of the General Geometry TWOTRAN Program,” LA-4432 (1970).
6) T. B. Fowler, D. R. Vondy and G. W. Cummingham: “Nuclear Reactor Analysis Code; CITATION,“ ORNL-TM-2496 (1969).
7) Y. Ishiguro: “PEACO-II: A Code for Calculation of Effective Cross Section in Heterogeneous Systems,” JAERI-M 5527 (1971).
8) K. Okumura: “COREBN: A Core Burn-up Calculation Module of SRAC2006,” JAEA-Data/Code 2007-003 (2007).
9) K. Shibata, *et al*.: “Japanese Evaluated Nuclear Data Library Version 3 Revision-3: JENDL-3.3,” *J. Nucl. Sci. Technol*. **39**, 1125 (2002) and Nuclear Data Center at JAEA, (online) available from < http://wwwndc.tokai-sc.jaea.go.jp/index.html > (accessed 2006-12-19).
10) (Eds.) A.Koning, R.Forrest, M.Kellett, R.Mills, H.Henrikson and Y.Rugama: “The JEFF-3.1 Nuclear Data Library,” JEFF Report 21 (2006), and OECD/NEA: “The JEFF-3.1 Project”, (online) available from < http://www.nea.fr/html/dbdata/JEFF/ > (accessed 2006-12-7).
11) M.B. Chadwick, P. Oblozinsky, M. Herman *et al*.: “ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology,” Nuclear Data Sheets, **107**, pp. 2931-3060 (2006), and NNDC: “Evaluated Nuclear Data File (ENDF)”, (online) available from < http://www.nndc.bnl.gov/exfor7/endf00.htm > (accessed 2006-12-19)
12) IAEA: PREPRO2004 Home Page, (online) available from < http://www-nds.iaea.org/ndspub/endf/prepro/ > (accessed 2006-12-6).
13) Cullen D.E.: “Program LINEAR (Version 79-1): linearize data in the evaluated nuclear data file/version B (ENDF/B) format,” UCRL-50400 (1979).
14) Cullen D.E.: “Program RECENT (Version 79-1): reconstruction of energy-dependent neutron cross section from resonance parameters in the ENDF/B format,” UCRL-50400 Vol.17 Part C

(1979).

15) Cullen D.E.: “Program SIGMA1 (Version 79-1): Doppler broaden evaluated neutron cross sections in the evaluated nuclear data file/version B (ENDF/B) format,” UCRL-50400 (1979). Vol.17 Part B (1979).
16) R. E. MacFarlane and D. W. Muir: “The NJOY Nuclear Data Processing System Version 91”, LA-12740-M, Los Alamos National Laboratory (1994), and Los Alamos National Laboratory: T2 Nuclear Information Service, (online) available from < http://t2.lanl.gov/ > (accessed 2006-12-7).
17) H. Takano, Y. Ishiguro, Y. Matsui: “TIMS-1: A Processing Code for Production of Group Constants of Heavy Resonance Nuclei,” JAERI 1267 (1980).
18) J. B. Scarborough: “Numerical Mathematical Analysis,” The Johns Hopkins Press, Baltimore (1962).
19) Y. Ishiguro, *et al.*: “Generalized Dancoff Factor in Complex Lattice Arrangement,” *J. Nucl. Sci. Technol.*, **22**, 853 (1985).
20) T. Tone: “A Numerical Study of Heterogeneity Effects in Fast Reactor Critical Assemblies,” *J. Nucl. Sci. Technol.*, **12**(8), 467 (1975).
21) Y. Ishiguro and H. Takano: *J. Nucl. Sci. Technol.*, **6**, 380 (1969).
22) P. H. Kier: “RIFF-RAFF, A Program for Computation of Resonance Integrals in a Two Region Cell,” ANL-7326 (1967).
23) G. I. Bell, G. E. Hansen and H. A. Sandmeir: *Nucl. Sci. Eng*. **28**, 376 (1967).
24) J. S. Durek, G. D. Joanou and E. L. Leshan: “GAM-I; A Consistent P1 Multigroup for the Calculation of Fast Neutron Spectra and Multigroup Constants,” GA-1850 (1961).
25) P. Benoist: “Theorie du Coefficient des Diffusion des Neutrons dans un Reseau Comportant des Cavites,” CEA-R 2278 (1964).
26) K. Tsuchihasi, Y. Ishiguro and K. Kaneko: “Double Heterogeneity Effect on Resonance Absorption in Very High Temperature Gas-Cooled Reactor,” *J. Nucl. Sci. Technol.*, **22**(1), 16 (1985).
27) K. M. Case, F. De Hoffman and G. Placzek: “Introduction to the Theory of Neutron Diffusion,” Los Alamos Scientific Lab. (1953).
28) T. Olsen: “Void Streaming in Sn Calculations,” *Nucl. Sci. Eng.*, **21**, 271 (1965).
29) K. Okumura, H. Akie: “Improvement and Extension of Burn-up Chain Models for the SRAC and MVP-BURN Codes,” to be published in JAEA-Data/Code (2007) [in Japanese]
30) Y. Nakahara, *et al.* : *Radiochimica Acta*, **50**, 141 (1990).
31) K. Okumura, T. Mori, N. Nakagawa and K. Kaneko, “Validation of a Continuous-Energy Monte Carlo Burn-up Code MVP-BURN and Its Application to Analysis of Post Irradiation

Experiment," *J. Nucl. Sci. Technol*, **37**, 128 (2000).

32) R. Chawla, R. Seiler and K. Gmur: "Effects of Fuel Enrichment on the Physics Characteristics of Plutonium-Fueled Light Water High Converter Reactors," *Nucl. Technol.*, **73**, 296 (1986).

33) K. Tsuchihashi : "Collision Probability in Two-Dimensional Lattice by Ray-Trace Method and its Applications to Cell Calculations," JAERI-M 85-034 (1985).

34) H. Honeck: "THERMOS; A Thermalization Transport Theory Code for Reactor Lattice Calculations," BNL-5826 (1961).

35) H. Takahashi: *J. Nuclear Energy*, A, **12**, 1 (1960).

36) K. Tsuchihashi and Y. Gotoh: *Nucl. Sci. Eng.*, **58**, 213 (1975).

37) E. Teuchert: *Nucleonik*, **11**, 68 (1968).

38) Y. Fukai : *J. Nucl. Energy*, A/B, **17**, 115 (1963).

39) L. Amyot and P. Benoist: *Nucl. Sci. Eng.*, **26**, 215 (1967) and C. Daolio: "PROCOPE; A Code to Evaluate Collision Probabilities in Pin Clusters and Infinite Rod Lattice," EUR 3296,e (1967).

40) H. Takahashi and T. Nakayama: "The First Flight Collision Probability in the Square and Hexagonal Lattice Systems," JAERI 1072 (1964).

41) H. Takahashi, T. Nakayama and T. Tsutsui: "Code GRAFA; An IBM-7044 FORTRAN IV Code for Calculation of the Neutron Spectrum for Square and Hexagonal Lattices," JAERI 1097 (1965).

42) I. Carlvik: "A Method for Calculating Collision Probabilities in General Cylindrical Geometry and Application to Flux Distributions and Dancoff Factors," Proc. Third Int. Conf. Peaceful Uses of Atomic Energy, Geneva, Switzerland, August 31- September 9, 1964, Vol.2, p.225, United Nations, New York (1965).

43) J. E. Beardwood: "PIJ; A Computer Programme for the Calculation of Collision Probabilities," AEEW-R440 (1966).

44) K. Tsuchihashi: "PATH-C; A Computer Program for the Calculation of Collision Probabilities in a Multi-region Cell," JAERI-memo 2984 (1968) [in Japanese].

45) K. Tsuchihashi: "CLUP; A Computer Program for the Calculation of Multi-region Multi-group Collision Probabilities in a Cluster Lattice," JAERI-memo 2984 (1968) [in Japanese].

46) K. Tsuchihashi: "CLUP77; A Fortran Program of Collision Probabilities for Square Clustered Assembly," JAERI 1196 (1971).

47) K. Tsuchihashi: "CLUPH; A Fortran Program of Collision Probabilities for Hexagonal Lattice and It's Application to VHTR," JAERI-M 9301 (1981).

48) R. Bonalumi: *Energia Nucleare*, **8**, 326 (1961).

49) Z. Schloemich: *Math. Phys.*, **4**, 390 (1859).

50) W. G. Bickley and J. Naylor: *Phylos. Mag.*, **20**, 343(1935).
51) I. I. Bondarenko Ed.: “Group Constants for Nuclear Reactor Calculations,” Consultant Bureau, New York (1964).
52) For example, G. I. Bell and S. Glasstone: “Nuclear Reactor Theory,” Van Nostrand Co. (1970).
53) R. Goldstein and E. R. Cohen: *Nucl. Sci. Eng.*,**13**, 132 (1962).
54) Y. Ishiguro: *Nucl. Sci. Eng.*, **32**, 422 (1968).
55) Y. Ishiguro, S. Inoue and H. Takano: *J.Nucl.Sci.Tecnol.*, **6**, 308 (1969).
56) M. M. Levine: *Nucl. Sci. Eng.*, **16**, 271 (1963).
57) D. C. Leslie, J. G. Hill, and A. Jonsson: *Nucl. Sci. Eng.*, **22**, 78 (1965).
58) H. H. Hummel and D. Okrent: “Reactivity Coefficients in Large Fast Power Reactors,” American Nuclear Society (1970).
59) K. Tsuchihashi, Y. Ishiguro and K. Kaneko: *Nucl. Sci. Eng.*, **73**, 164 (1980).
60) J. Dwork *et al.*: “Self-shielding Factors for Infinitely Long, Hollow Cylinders,” KAPL-1262 (1955).
61) For example, R. J. Stammler and M. J. Abbate: “Methods of Steady-State Reactor Physics in Nuclear Design,” Academic Press, London (1982).
62) D. Meneghetti: Proc. Int. Conf. Fast Critical Assemblies and Their Analysis, ANL-7320, p.377, (1966).
63) R. Chawla *et al.*: *Nucl. Technol.*, **67**, 360(1984).
64) W. Rothenstein : *Nucl. Sci. Eng.*, **13**, 132(1962).
65) D. C. Leslie *et al.*: ibid., **22**, 78(1965).
66) P. H. Kier and A. A. Robba: “RABBLE, A Program for Computation of Resonance Integrals in Multiregion Reactor Cells,” ANL 7645 (1975).
67) Y. Ishiguro and H. Takano: “PEACO: A Code for Calculation of Group Constants of Resonance Energy Region in Heterogeneous Systems,” JAERI 1219 (1971).
68) Y. Ishiguro: *Nucl. Sci. Eng.*, **51**, 441 (1973).
69) J. B. Scarborough: “Numerical Mathematical Analysis,” The Johns Hopkins Press, Baltimore (1962).
70) D. C. Leslie and A. Jonsson: *Nucl. Sci. Eng.*, **23**, 272 (1965).
71) H. Takano: “MCROSS-2; A Code for Calculation of Microscopic and Effective Cross Sections,” JAERI-M 4721 (1972).
72) L. W. Nordheim: Symposia Appl. Math., XI, 58 (1961).
73) M. Segev: *Nucl. Sci. Eng.*, **81**, 151 (1982).
74) R. K. Lane, L. W. Nordheim and J. B. Sampson: *Nucl. Sci. Eng.*, **14**, 390 (1962).

75) K. Tasaka : “DCHAIN: Code for Analysis of Build-up and Decay of Nuclides,” JAERI 1250 (1977) [in Japanese].
76) Japanese Nuclear Data Committee and Nuclear Data Center: “CHART OF THE NUCLIDES 2004,” Japan Atomic Energy Research Institute (2006).
77) K. Tasaka, *et.al.*: “JNDC Nuclear Data Library of Fission Products - Second Version -,” JAERI 1320 (1990).
78) T. Nakagawa, *et al.*: “Japanese Evaluated Nuclear Data Library Version 3 Revision-2: JENDL-3.2,” *J. Nucl. Sci. Technol.*, **32**, 1259 (1995).
79) OECD/NEA Data Bank: “The JEFF-3.0 Nuclear Data Library, JEFF Report 19,” (2005). and OECD/NEA: “Nuclear Data Services - JEFF and EFF projects,” (online) available from < http://www.nea.fr/html/dbdata/projects/nds_jef.htm > (accessed 2006-12-19).
80) OECD/NEA Data Bank: “The JEF-2.2 Nuclear Data Library, JEFF Report 17,” (2000).
81) National Nuclear Data Center: “Evaluated Nuclear Data File (ENDF),” (online) available from < http://www.nndc.bnl.gov/exfor3/endf00.htm > (accessed 2006-12-19).
82) (Eds.) P. F. Rose: “ENDF-201, ENDF/B-VI Summary Documentation,” BNL-NCS-17541, 4th Edition (1991).
83) (Eds.) D. Garber: “ENDF/B Summary Documentation,” BNL-17541, 2nd Edition (1975).

国際単位系（SI）

表１．SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd

表２．基本単位を用いて表されるSI組立単位の例

組立量	SI 基本単位	
	名称	記号
面積	平方メートル	m^2
体積	立法メートル	m^3
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s^2
波数	毎メートル	m-1
密度（質量密度）	キログラム毎立法メートル	kg/m^3
質量体積（比体積）	立法メートル毎キログラム	m^3/kg
電流密度	アンペア毎平方メートル	A/m^2
磁界の強さ	アンペア毎メートル	A/m
（物質量の）濃度	モル毎立方メートル	mol/m^3
輝度	カンデラ毎平方メートル	cd/m^2
屈折率	（数の）1	1

表５．SI 接頭語

乗数	接頭語	記号	乗数	接頭語	記号
10^{24}	ヨタ	Y	10^{-1}	デシ	d
10^{21}	ゼタ	Z	10^{-2}	センチ	c
10^{18}	エクサ	E	10^{-3}	ミリ	m
10^{15}	ペタ	P	10^{-6}	マイクロ	μ
10^{12}	テラ	T	10^{-9}	ナノ	n
10^{9}	ギガ	G	10^{-12}	ピコ	p
10^{6}	メガ	M	10^{-15}	フェムト	f
10^{3}	キロ	k	10^{-18}	アト	a
10^{2}	ヘクト	h	10^{-21}	ゼプト	z
10^{1}	デカ	da	10^{-24}	ヨクト	y

表３．固有の名称とその独自の記号で表されるSI組立単位

組立量	SI 組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン(a)	rad		$m \cdot m^{-1}=1$(b)
立体角	ステラジアン(a)	sr(c)		$m^2 \cdot m^{-2}=1$(b)
周波数	ヘルツ	Hz		s^{-1}
力	ニュートン	N		$m \cdot kg \cdot s^{-2}$
圧力，応力	パスカル	Pa	N/m^2	$m^{-1} \cdot kg \cdot s^{-2}$
エネルギー，仕事，熱量	ジュール	J	$N \cdot m$	$m^2 \cdot kg \cdot s^{-2}$
工率，放射束	ワット	W	J/s	$m^2 \cdot kg \cdot s^{-3}$
電荷，電気量	クーロン	C		$s \cdot A$
電位差（電圧），起電力	ボルト	V	W/A	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$
静電容量	ファラド	F	C/V	$m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$
電気抵抗	オーム	Ω	V/A	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$
コンダクタンス	ジーメンス	S	A/V	$m^{-2} \cdot kg^{-1} \cdot s^3 \cdot A^2$
磁束	ウエーバ	Wb	$V \cdot s$	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-1}$
磁束密度	テスラ	T	Wb/m^2	$kg \cdot s^{-2} \cdot A^{-1}$
インダクタンス	ヘンリー	H	Wb/A	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-2}$
セルシウス温度	セルシウス度(d)	℃		K
光束	ルーメン	lm	$cd \cdot sr$(c)	$m^2 \cdot m^{-2} \cdot cd=cd$
照度	ルクス	lx	lm/m^2	$m^2 \cdot m^{-4} \cdot cd=m^{-2} \cdot cd$
（放射性核種の）放射能	ベクレル	Bq		s^{-1}
吸収線量，質量エネルギー分与，カーマ	グレイ	Gy	J/kg	$m^2 \cdot s^{-2}$
線量当量，方向性線量当量，個人線量当量，組織線量当	シーベルト	Sv	J/kg	$m^2 \cdot s^{-2}$

(a)ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときのいくつかの用例は表４に示されている。
(b)実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号“１”は明示されない。
(c)測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。
(d)この単位は、例としてミリセルシウス度m℃のようにSI接頭語を伴って用いても良い。

表４．単位の中に固有の名称とその独自の記号を含むSI組立単位の例

組立量	SI 組立単位		
	名称	記号	SI 基本単位による表し方
粘度	パスカル秒	Pa・s	$m^{-1} \cdot kg \cdot s^{-1}$
力のモーメント	ニュートンメートル	N・m	$m^2 \cdot kg \cdot s^{-2}$
表面張力	ニュートン毎メートル	N/m	$kg \cdot s^{-2}$
角速度	ラジアン毎秒	rad/s	$m \cdot m^{-1} \cdot s^{-1}=s^{-1}$
角加速度	ラジアン毎平方秒	rad/s^2	$m \cdot m^{-1} \cdot s^{-2}=s^{-2}$
熱流密度，放射照度	ワット毎平方メートル	W/m^2	$kg \cdot s^{-3}$
熱容量，エントロピー	ジュール毎ケルビン	J/K	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$
質量熱容量（比熱容量），質量エントロピー	ジュール毎キログラム毎ケルビン	J/(kg・K)	$m^2 \cdot s^{-2} \cdot K^{-1}$
質量エネルギー（比エネルギー）	ジュール毎キログラム	J/kg	$m^2 \cdot s^{-2} \cdot K^{-1}$
熱伝導率	ワット毎メートル毎ケルビン	W/(m・K)	$m \cdot kg \cdot s^{-3} \cdot K^{-1}$
体積エネルギー	ジュール毎立方メートル	J/m^3	$m^{-1} \cdot kg \cdot s^{-2}$
電界の強さ	ボルト毎メートル	V/m	$m \cdot kg \cdot s^{-3} \cdot A^{-1}$
体積電荷	クーロン毎立方メートル	C/m^3	$m^{-3} \cdot s \cdot A$
電気変位	クーロン毎平方メートル	C/m^2	$m^{-2} \cdot s \cdot A$
誘電率	ファラド毎メートル	F/m	$m^{-3} \cdot kg^{-1} \cdot s^4 \cdot A^2$
透磁率	ヘンリー毎メートル	H/m	$m \cdot kg \cdot s^{-2} \cdot A^{-2}$
モルエネルギー	ジュール毎モル	J/mol	$m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$
モルエントロピー，モル熱容量	ジュール毎モル毎ケルビン	J/(mol・K)	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1} \cdot mol^{-1}$
照射線量（X線及びγ線）	クーロン毎キログラム	C/kg	$kg^{-1} \cdot s \cdot A$
吸収線量率	グレイ毎秒	Gy/s	$m^2 \cdot s^{-3}$
放射強度	ワット毎ステラジアン	W/sr	$m^4 \cdot m^{-2} \cdot kg \cdot s^{-3}=m^2 \cdot kg \cdot s^{-3}$
放射輝度	ワット毎平方メートル毎ステラジアン	$W/(m^2 \cdot sr)$	$m^2 \cdot m^{-2} \cdot kg \cdot s^{-3}=kg \cdot s^{-3}$

表６．国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h =60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	1°=(π/180) rad
分	’	1’=(1/60)°=(π/10800) rad
秒	”	1”=(1/60)’=(π/648000) rad
リットル	l、L	1l=1 $dm^3=10^{-3}m^3$
トン	t	$1t=10^3$ kg
ネーパ	Np	1Np=1
ベル	B	1B=(1/2)ln10(Np)

表７．国際単位系と併用されこれに属さない単位でSI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位であらわされる数値
電子ボルト	eV	$1eV=1.60217733(49) \times 10^{-19}J$
統一原子質量単位	u	$1u=1.6605402(10) \times 10^{-27}kg$
天文単位	ua	$1ua=1.49597870691(30) \times 10^{11}m$

表８．国際単位系に属さないが国際単位系と併用されるその他の単位

名称	記号	SI 単位であらわされる数値
海里		1海里=1852m
ノット		1ノット=1海里毎時=(1852/3600)m/s
アール	a	1 a=1 $dam^2=10^2m^2$
ヘクタール	ha	1 ha=1 $hm^2=10^4m^2$
バール	bar	1 bar=0.1MPa=100kPa=1000hPa=10^5Pa
オングストローム	Å	1 Å=0.1nm=10^{-10}m
バーン	b	1 b=100$fm^2=10^{-28}m^2$

表９．固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	1 erg=10^{-7} J
ダイン	dyn	1 dyn=10^{-5}N
ポアズ	P	1 P=1 dyn・s/cm^2=0.1Pa・s
ストークス	St	1 St =1$cm^2/s=10^{-4}m^2/s$
ガウス	G	1 G ^10^{-4}T
エルステッド	Oe	1 Oe ^(1000/4π)A/m
マクスウェル	Mx	1 Mx ^10^{-8}Wb
スチルブ	sb	1 sb =1$cd/cm^2=10^4cd/m^2$
ホト	ph	1 ph=10^4lx
ガル	Gal	1 Gal =1$cm/s^2=10^{-2}m/s^2$

表10．国際単位に属さないその他の単位の例

名称	記号	SI 単位であらわされる数値
キュリー	Ci	1 Ci=3.7×10^{10}Bq
レントゲン	R	1 R = 2.58×10^{-4}C/kg
ラド	rad	1 rad=1cGy=10^{-2}Gy
レム	rem	1 rem=1 cSv=10^{-2}Sv
X線単位		1X unit=1.002×10^{-4}nm
ガンマ	γ	1γ=1 nT=10^{-9}T
ジャンスキー	Jy	1 Jy=$10^{-26}W \cdot m^{-2} \cdot Hz^{-1}$
フェルミ		1 fermi=1 fm=10^{-15}m
メートル系カラット		1 metric carat = 200 mg = 2×10^{-4}kg
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリー	cal	
ミクロン	μ	1 μ =1μm=10^{-6}m

（第７版，1998年改訂）