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DEVELOPMENT OF BERMUDA : A RADIATION TRANSPORT CODE SYSTEM PART II. GAMMA RAYS TRANSPORT CODES

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Development of BERMUDA : A Radiation Transport Code System Part II. Gamma Rays Transport Codes

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A radiation transport code system BERMUDA has been developed for one-, two- and three-dimensional geometries. Purpose of the development is to establish a basis of an accurate shielding calculation method for general use. The time-independent transport equation is numerically solved using a direct integration method in a multigroup model, to obtain spatial, angular and energy distributions of neutron, gamma rays or adjoint neutron flux. In 1992, the neutron transport codes were reported in JAERI 1327 as Part I. In the present report as Part II, development of gamma rays transport codes is reported. As described in Part I, the spherical harmonics expansion is not used in representing anisotropy of both angular flux and scattering cross sections. Group-angle transfer matrix is calculated by numerically integrating the Klein-Nishina formula for Compton scattering, taking energy-angle correlation into account. Pair production and annihilation of electrons are also contained in the matrix. A first collision source method is used for a case of point source. Angular flux distribution is obtained by integrating the transport equation over the line segment along each angular discrete ordinate at each spatial mesh point. A fine energy grid (subgroup having equal energy width) method is used, with a rebalancing scheme con-

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cerning the number of gain and loss of photons over each coarse mesh region and also in each energy grid. Energy range of photons is from 14 MeV to 10 keV. As to group constants, three kinds of libraries with photon energy group structure up to 41 groups have been prepared to contain total (attenuation) cross sections and secondary gamma rays production constants from each of neutron groups. A benchmark test has been performed by analyzing a secondary gamma-ray heating experiment performed at the FNS facility in JAERI. In the present report, the calculational methods of photon transport in the BERMUDA code system are briefly described. As a main purpose of this report, input data specifications, job control languages and output data are given as a user's manual for the following four gamma rays transport codes:

BERMUDA-1DG	: sphere, slab	(S_{20})
BERMUDA-2DG	: cylinder	(S_8)
BERMUDA-2DG-S16	: cylinder	(S_{16})
BERMUDA-3DG	: rectangular parallelpiped	(S_8)

Development of adjoint neutron transport codes will be reported as Part Ⅲ.

Keywords: BERMUDA, Radiation Transport, Shielding, Code System, Direct Integration Method, Energy Group, Gamma Rays, Compton Scattering, Anisotropy, Angular Discrete Ordinates, Secondary Gamma-ray Heating, Pair Production, Annihilation, Electron

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放射線輸送コードシステムＢＥＲＭＵＤＡの開発
第Ⅱ部　ガンマ線輸送コード

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（1993年６月14日受理）

高精度の遮蔽計算を行うコードシステムの完成を目標に，その計算手法の基礎を確立するため，１～３次元の各形状に対する放射線輸送コードシステムＢＥＲＭＵＤＡを開発した。本コードシステムでは直接積分法と，エネルギーに関する多群モデルを組合わせて定常状態での輸送方程式を数値的に解き，中性子，ガンマ線あるいは随伴中性子の各線束の空間，角度，エネルギー分布を求めている。1992年に第Ｉ部中性子輸送コードの開発がJAERI 1327として報告された。本報告書は第Ⅱ部としてガンマ線輸送コードの開発について報告している。第Ｉ部に述べたように，線束や散乱断面積の非等方性の表現に球面調和関数展開を用いていない。コンプトン散乱による群・角度遷移マトリックスの算出には，エネルギーと散乱角の相関を考慮して，クライン－仁科の公式の数値積分を行う。電子対の生成と消滅もこのマトリックスに含めた。さらに，点線源の場合は一回散乱源を求めてから輸送方程式を解く方法を用いている。線束の空間・角度分布は各格子点で各角度分点の方向へ輸送方程式を積分し，エネルギー群を等分割した微細群毎に，領域毎の粒子バランスが成り立つように規格化を行いつつ求める。光子のエネルギー範囲は14MeVから10keVまでとした。群定数ライブラリーとして，41群以内の群構造のものが３種類用意された。これらのライブラリーには光子の減衰全断面積及び中性子各群からの二次ガンマ線生成定数が群毎核種毎に格納されている。コードのベンチマークテストはＦＮＳを用いて行った二次ガンマ線発熱分布測定実験の解析により行った。本報告書ではＢＥＲＭＵＤＡコードシステムでの光子輸送計算法について概説すると共に，主目的としては次の４個のガンマ線輸送コード

ＢＥＲＭＵＤＡ－１ＤＧ　　（１次元球，平板体系，S_{20}）
ＢＥＲＭＵＤＡ－２ＤＧ　　（２次元円柱体系，　S_8）
ＢＥＲＭＵＤＡ－２ＤＧ－Ｓ１６（２次元円柱体系，　S_{16}）
ＢＥＲＭＵＤＡ－３ＤＧ　　（３次元直方体体系，　S_8）

の使用マニュアルとして，ジョブ制御文と入力データの準備，更に出力データの概要について述べている。随伴中性子輸送コードについては第Ⅲ部で報告する。

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1. Introduction

The radiation transport code system BERMUDA consists of three subsystems as:

(1) Neutron transport codes,
(2) Gamma rays transport codes and
(3) Adjoint neutron transport codes.

Out of these, four neutron transport codes were reported in JAERI 1327 (Ref.1) as Part Ⅰ in 1992. The present report is written as Part Ⅱ for the gamma rays transport codes.

Almost all of the numerical methods to solve the neutron transport equation are commonly used in the gamma rays transport codes. However, there exist several characteristic features in photon transport codes such as:

(a) A photon has not 'mass', but 'energy' determined by its frequency,
(b) Energy-angle transfer matrix is obtained by Compton scattering law represented by Klein-Nishina formula,
(c) The production and annihilation of electron-positron pair are also added to the matrix. The emitted photons are treated as isotropic and monoenergetic (two photons having energy of 511keV) and
(d) Besides independent photon sources like those of radioisotopes, the major sources can be given as secondary gamma rays from neutron-nucleus reactions mainly by (n,γ), $(n,n'\gamma)$ and $(n,\text{fission}\,\gamma)$ processes.

We have developed four computer codes for obtaining space, angle and energy distributions of photon flux in one-, two- and three-dimensional typical geometries. This report is written as a usage manual for these codes.

In Chapter 2, the group constants library for BERMUDA gamma rays calculation is briefly described. The characteristic features to solve the photon transport equation in the present version of the code system are introduced in Chapter 3. A simple validity test is also given by secondary gamma-ray

heating calculation. Chapter 4 is a guide for users to prepare input data and the job control languages for the FACOM/VP2600 computer. Also, a brief description is given about the output data on printer or disk.

The adjoint neutron transport codes in the BERMUDA code system will be reported as Part Ⅲ.

2. Group Constants Library

The group constants libraries for the BERMUDA gamma rays subsystem contain: (1) secondary gamma rays production constants with neutron-nucleus reactions, and (2) microscopic total cross sections of atoms for making up total attenuation coefficients for gamma rays. Both of these data are prepared for each energy group of gamma rays with a group constants processing code PROF-GROUCH-G/B[2].

The total cross section in the library is evaluated as the sum of the cross sections of photoelectric effect, pair production and Compton scattering.

There are three libraries of gamma rays group constants prepared for BERMUDA test calculations;

(a) J2585.BERM1DG.DATA

36 groups, 30 nuclides.

Secondary gamma rays production data sources are ENDF/B-Ⅳ[3] and ENDL-78[4]. Number of neutron groups is 120, and neutron transport calculation should be performed using J2585.BERMUDA1.DATA or J2585.BERMUDAJ.DATA.

(b) J2585.BERM125S.B4G.DATA

40 groups, 12 nuclides.

Secondary gamma rays production data source is ENDF/B-Ⅳ. Number of neutron groups is 125, and neutron transport calculation should be performed using J2585.BERM125S.B4.DATA.

(c) J449B.BERM41G.DATA

41 groups, 20 nuclides.

Secondary gamma rays production data source is JENDL-3[5]. Number of neutron groups is 125, and neutron transport calculation should be performed using J449B.BERM125X.DATA.

In the following, details are given only for the newest library J449B.BERM41G.DATA.

2.1 Nuclides, Code Numbers and Atomic Numbers

The twenty nuclides in the library J449B.BERM41G.DATA are as follows.

The code number is used as identification number when the atomic density is input to BERMUDA. The atomic number(Z) is obtained by dividing the code number by 100 in integer.

Order in Library	Nuclide Name	Code Number	Atomic Number
1	H	117	1
2	^{6}Li	307	3
3	^{7}Li	317	3
4	Be	407	4
5	^{10}B	507	5
6	^{11}B	517	5
7	C	607	6
8	N	707	7
9	O	807	8
10	Na	1107	11
11	Mg	1207	12
12	Al	1307	13
13	Si	1407	14
14	Ca	2007	20
15	Cr	2407	24
16	Mn	2507	25
17	Fe	2607	26
18	Ni	2807	28
19	Mo	4207	42
20	Pb	8207	82

2.2 Energy Group Structure

The neutron energy group structure in making the secondary gamma rays production matrix is 125 groups and their energy boundaries are same as in J449B.BERM125X.DATA[1]. This production matrix is evaluated for each nuclide considering up to 20 kinds of neutron-nucleus reactions at the maximum.

The gamma rays energy group structure is 41 groups from 14MeV to 10keV as follows. In case of gamma rays, the mid-point is defined as arithmetical mean value of the upper and lower boundary energies.

Group No.	Upper Energy	Lower Energy	Middle Energy
1	14.0(MeV)	12.0(MeV)	13.0(MeV)
2	12.0	10.0	11.0
3	10.0	9.00	9.50
4	9.00	8.00	8.50
5	8.00	7.50	7.75
6	7.50	7.00	7.25
7	7.00	6.50	6.75
8	6.50	6.00	6.25
9	6.00	5.50	5.75
10	5.50	5.00	5.25
11	5.00	4.50	4.75
12	4.50	4.00	4.25
13	4.00	3.50	3.75
14	3.50	3.00	3.25
15	3.00	2.50	2.75
16	2.50	2.25	2.375
17	2.25	2.00	2.125
18	2.00	1.75	1.875
19	1.75	1.50	1.625
20	1.50	1.375	1.4375
21	1.375	1.25	1.3125
22	1.25	1.125	1.1875
23	1.125	1.00(MeV)	1.0625(MeV)
24	1.00(MeV)	900(keV)	950(keV)
25	900(keV)	800	850
26	800	700	750
27	700	600	650
28	600	512	556
29	512	510	511
30	510	450	480
31	450	400	425
32	400	300	350
33	300	200	250

34	200	150	175
35	150	100	125
36	100	80.0	90.0
37	80.0	60.0	70.0
38	60.0	45.0	52.5
39	45.0	30.0	37.5
40	30.0	20.0	25.0
41	20.0	10.0	15.0

2.3 Data Arrangements in the Library

The library J449B.BERM41G.DATA consists of 167 binary records as follows:

(1) The first header record is

NMAXL, MMAXL, (EUPN(N), N＝1, NMAXL+1), (EMIDN(N), N＝1, NMAXL),
(DELUN(N), N＝1, NMAXL), (NCODEL(M), M＝1, MMAXL), NGMAX, MXREAC,
(EUP(I), I＝1, NGMAX+1), (EMID(I), I＝1, NGMAX), (DELU(I), I＝1, NGMAX),

where NMAXL : number of neutron energy groups (＝125),
MMAXL : number of nuclides in the library (＝20),
EUPN : neutron upper energy boundary (eV)[1],
EMIDN : neutron group mid-point in lethargy (eV)[1],
DELUN : neutron group lethargy width[1],
NCODEL : nuclide code number,
NGMAX : number of gamma rays energy groups (＝41),
MXREAC : dummy,
EUP : gamma rays upper energy boundary (eV),
EMID : gamma rays group mid-point in energy (eV) and
DELU : gamma rays group lethargy width (dummy).

(2) The next 125 records are secondary gamma rays production constants for neutron groups N (N＝1, …, 125):

((GPROD(I, M, N), I＝1, NGMAX), M＝1, MMAXL),

where GPROD : secondary gamma rays production constant (summed up 'up to 20' kinds of neutron-nucleus reactions; neutron cross section is already multiplied to production constant for each reaction),

I : gamma rays group no.,

M : nuclide no. and

N : neutron group no.

(3) The next 41 records are total cross sections of nuclides for gamma rays groups I (I＝1,…,41):

(SST(I,M),M＝1,MMAXL),

where SST : microscopic total cross section σ_t for gamma rays (barn/atom),

I : gamma rays group no. and

M : nuclide no.

3. Numerical Method to Solve Photon Transport Equation

The time-independent transport equation in a usual multigroup model is written as[1)]

$$\vec{\Omega} \cdot \mathrm{grad}\,\phi^i(\vec{r}, \vec{\Omega}) + \Sigma_t{}^i(\vec{r})\,\phi^i(\vec{r}, \vec{\Omega}) = q^i(\vec{r}, \vec{\Omega}). \qquad (3.1)$$

Symbols in Eq.(3.1) are as follows:

- $\vec{\Omega}$: unit direction vector drawn from the spatial point $\vec{r}$,
- $\cdot$: sign for inner product of vectors, i.e. $\vec{\Omega} \cdot$ means direction cosine between directions of $\vec{\Omega}$ and gradient operator,
- $\vec{r}$: coordinate of spatial point,
- i : group index of gamma rays energy,
- $\phi^i(\vec{r}, \vec{\Omega})$: angular flux of gamma rays at $(\vec{r}, \vec{\Omega})$ for group i, that is, the integrated value of $\phi(\vec{r}, E, \vec{\Omega})$ over the energy group width $\Delta E_i = [E_{i+1}, E_i]$ (photon/(cm^2 · sec · sr)),
- $\Sigma_t{}^i(\vec{r})$: macroscopic total cross section for gamma rays (cm^{-1}) ($\Sigma_t{}^i(\vec{r}) = \sum_m N^m(\vec{r})\,\sigma_t{}^{mi}$, where $\sigma_t{}^{mi}$ is an averaged value over the group i and given in Chapter 2) and
- $N^m(\vec{r})$: atomic number density (10^{24}cm^{-3}) of nuclide m in the medium at $\vec{r}$.

The right hand side of Eq.(3.1) is the photon source and is separated as follows:

$$q^i(\vec{r}, \vec{\Omega}) = q_n{}^i(\vec{r}, \vec{\Omega}) + q_{pp}{}^i(\vec{r}, \vec{\Omega}) + q_c{}^i(\vec{r}, \vec{\Omega}) + S^i(\vec{r}, \vec{\Omega}), \qquad (3.2)$$

where
- $q_n{}^i$: secondary gamma rays source generated by reaction of neutron with nucleus in a medium (Section 3.1),
- $q_{pp}{}^i$: source having energy of 0.511MeV generated by electron-positron pair production and annihilation (Section 3.2),
- $q_c{}^i$: source by Compton scattering (Section 3.3) and
- S^i : fixed gamma rays source (input data).

These sources are all defined as integrated value over the photon energy group range ΔE_i.

3.1 Secondary Gamma Rays Source

The neutron-induced secondary gamma rays production constants GPROD given in Chapter 2 is defined as the product of (a) number of photons generated by a reaction of j_n-th group neutron and a nuclide and (b) neutron microscopic cross section of the nuclide for the reaction. As to the kind of reactions, the products are already summed up. The dimension of GPROD is [photons/reaction] × [barn/atom] . Then, by multiplying atomic number density of a medium and neutron scalar flux to GPROD, we have photon generation rate per unit volume and per unit time (photons/(cm^3 · sec)).

Assuming this photon source to emit isotropically, the q_n in the right hand side of Eq.(3.2) is given as

$$q_n{}^i(\vec{r}, \vec{\Omega}) = (1/4\pi) \sum_{jn=1}^{IMAXN} \Phi^{jn}(\vec{r}) \sum_m N^m(\vec{r}) GPROD^{m,\, jn \to i}, \qquad (3.3)$$

where $\Phi(\vec{r})$ is neutron scalar flux obtained by the BERMUDA neutron transport calculation.[1)]

3.2 Pair Production and Annihilation of Electrons

When the energy of photons is greater than 1.022MeV($=2m_ec^2$), some of photons are absorbed by material atom in the rate according to pair production cross section σ_{pp}. Then a pair of electron and positron is created. These particles immediately annihilate and emit a part of their energy as two photons of 0.511MeV.

The cross section σ_{pp} is calculated in BERMUDA using the mid-energy of i-th group (EMID(i)) and atomic number Z^m of nuclide m as follows:[6)]

(i) $E^i \leqq 1.022\text{MeV}$

$$\sigma_{pp}^{mi} = 0.,$$

(ii) $1.022\text{MeV} < E^i < 2\text{MeV}$

$$\sigma_{pp}^{mi} = (1/137)(Z^m r_o)^2 (2\pi/3)\,[(k-2)/k]^3 \times [1+(1/2)\rho+(23/40)\rho^2+(11/60)\rho^3+(29/960)\rho^4] \text{ and}$$

(iii) $E^i \geqq 2\text{MeV}$

$$\sigma_{pp}^{mi} = (1/137)(Z^m r_o)^2 (a_o+a_1x+a_2x^2+a_3x^3).$$

The symbols used are:

r_o : classical radius of electron ($r_o^2 = 7.939827\times10^{-2}$barn),

$k = E^i/m_ec^2$,

m_e : electron rest mass ($m_ec^2 = 0.511006\times10^6$eV),

$\rho = (2k-4)/(2+k+2\sqrt{2k})$,

$x = (2/k)^2$,

$a = -218/27+(28/9)y$,

$a_1 = (\pi^2/6+2\zeta-7/2)+(6-\pi^2/3)y-y^2+(2/3)y^3$,

$a_2 = -1/8-(3/16)y$,

$a_3 = 77/27.512-(29/9.256)y$,

$y = \ln(2k)$ and

$\zeta = \sum_{n=1}^{\infty} n^{-3} = 1.2020569.$

Assuming these two photons of 0.511MeV are emitted isotropically, q_{pp} in Eq.(3.2) is given as

$$q_{PP}{}^{i}(\vec{r},\vec{\Omega}) = (2/4\pi)\,\delta_{i,29}\sum_{j=1}^{23}\Psi^{j}(\vec{r})\sum_{m}N^{m}(\vec{r})\,\sigma_{PP}{}^{mj},$$

where $\Psi^{j}(\vec{r})$: gamma rays scalar flux at $\vec{r}$ for group j,

$$= \sum_{n'}\Delta\vec{\Omega}_{n'}\,\phi^{j}(\vec{r},\vec{\Omega}_{n'}),$$

$\vec{\Omega}_{n'}$: angular discrete ordinate[1],

$\Delta\vec{\Omega}_{n'}$: weight for angular integration[1] and

δ_{ij} : Kronecker's delta.

Then we can write

$$q_{PP}{}^{j\to i,\,n'\to n}(\vec{r}) = (1/2\pi)\,\delta_{i,29}\Delta\vec{\Omega}_{n'}\,\phi^{j}(\vec{r},\vec{\Omega}_{n'})\,\Sigma_{PP}{}^{j}(\vec{r}),$$

From this equation, obtained is an expression for group-angle transfer kernel for pair production,

$$K_{PP}{}^{j\to i,\,n'\to n}(\vec{r}) = (1/2\pi)\,\delta_{i,29}\Delta\vec{\Omega}_{n'}\,\Sigma_{PP}{}^{j}(\vec{r}) \qquad (3.4)$$

and $$q_{PP}{}^{i}(\vec{r},\vec{\Omega}_{n}) = \sum_{j=1}^{i}\sum_{n'}\phi^{j}(\vec{r},\vec{\Omega}_{n'})\,K_{PP}{}^{j\to i,\,n'\to n}(\vec{r}).$$

3.3 Compton Scattering

The term q_c in Eq.(3.2) is given as

$$q_c{}^i(\vec{r},\vec{\Omega}) = [\sum_m N^m(\vec{r})Z^m]\sum_{j=1}^{I}\int d\vec{\Omega}'\int_{\Delta E_j} dE'\,\phi^j(\vec{r},\vec{\Omega}')/\Delta E_j \times$$

$$\times\int_{\Delta E_i} dE\,\sigma(E'\to E,\vec{\Omega}'\to\vec{\Omega}). \qquad (3.5)$$

The double-differential cross section $\sigma(E'\to E,\vec{\Omega}'\to\vec{\Omega})$ is given by Klein-Nishina formula in the averaged form with respect to polarization of photon waves,[7)～9)]

$$\sigma(E'\to E,\vec{\Omega}'\to\vec{\Omega}) = (1/2)r_o{}^2(E/E')^2(E'/E+E/E'-1+\xi^2)$$

$$\times\delta(1-\xi+\lambda'-\lambda)\left|d\lambda/dE\right|, \qquad (3.6)$$

where $\lambda = m_e c^2/E$, $\lambda' = m_e c^2/E'$ and
$\xi = \cos\Theta = (\vec{\Omega}\cdot\vec{\Omega}')$.

From Eq.(3.5), Compton scattering kernel is defined as

$$q_c{}^i(\vec{r},\vec{\Omega}) = \sum_{j=1}^{I}\sum_{n'}\phi^j(\vec{r},\vec{\Omega}_{n'})K_c{}^{j\to i,\,n'\to n}(\vec{r}),$$

where

$$K_c{}^{j\to i,\,n'\to n}(\vec{r}) = [\sum_m N^m(\vec{r})Z^m]\int_{\Delta\vec{\Omega}_{n'}} d\vec{\Omega}'\int_{\Delta E_j}(dE'/\Delta E_j)\int_{\Delta E_i} dE\,\sigma(E'\to E,\vec{\Omega}'\to\vec{\Omega}_n).$$

Omitting m, $\sum_m$, $N^m(\vec{r})$ and Z^m for simplicity, and using Eq.(3.6),

$$K_c{}^{j\to i,\,n'\to n} = \int_{\Delta\vec{\Omega}_{n'}} d\vec{\Omega}'\int_{\Delta E_j}(dE'/\Delta E_j)\int_{\Delta E_i} dE(1/2)r_o{}^2(E/E')^2(E'/E+E/E'-1+\xi^2)$$

$$\times\delta(1-\xi+\lambda'-\lambda)(m_e c^2/E^2)$$

$$= (1/2) r_o^2 m_e c^2 \int_{\Delta \vec{\Omega}_{n'}} d\vec{\Omega}' \int_{\Delta E_j} (dE'/\Delta E_j) \int_{\Delta E_i} dE/E'^2$$

$$\times (E'/E + E/E' - 1 + \xi^2)\, \delta(1 - \xi + \lambda' - \lambda).$$

By Eq. (3.15) in Ref.1, $\int d\vec{\Omega}'$ can be written as $\int_{-1}^{1} d\xi \int_{0}^{2\pi} d\phi$. And using $\Delta\phi_{n'nm'}$ also defined in Ref.1, K_c finally becomes

$$K_c^{j \to i,\, n' \to n} = (1/2) r_o^2 m_e c^2 \int_{\Delta E_j} dE'/(E'^2 \Delta E_j) \int_{\Delta E_i} dE (E'/E + E/E' - 1 + \xi^2)$$

$$\times \Delta\phi_{n'nm'}\, \bar{\delta}(\xi, \xi_{m'}), \qquad (3.7)$$

where $\xi = 1 + \lambda' - \lambda$,

$$\Delta\phi_{n'nm'} = \int_{-1}^{1} d\xi\, \delta(\xi - \xi_{m'}) \int_{\Delta \vec{\Omega}_{n'}} d\phi_n ,$$

$$\xi_{m'} = \cos\Theta_{m'} ,$$

$\Theta_{m'} = (\pi/80)(m' - 1/2)$ $(m' = 1, \cdots, 80)$ and

the sign $\bar{\delta}$ means that m' in the table of $\Delta\phi_{n'nm'}$ is picked out and used, if ξ happens to fall in the fine interval of $\xi_{m'}$.[1)]

Equation(3.7) is numerically integrated with respect to E and E'. For given E, the range of E' is restricted by relations $\xi = 1 + \lambda' - \lambda$ and $-1 \leqq \xi \leqq 1$ as

$$E'_{max} = E/(1 - 2E/m_e c^2) \text{ and}$$

$$E'_{min} = E,$$

where $E'_{max} = 14$MeV is adopted when $1 - 2E/m_e c^2 \leqq 0$ or $E'_{max} > 14$MeV. Then, actual range [E'] for E' numerical integration is given,

$$[E'] = \Delta E_j \cap [E'_{min}, E'_{max}] .$$

Other details (such as treatment when j=i) is completely analogous as in case of neutron.[1)]

For given E', actual range [E] for E numerical integration is given as

$$E_{max} = E',$$

$$E_{min} = E'/(1+2E'/m_e c^2) \text{ and}$$

$$[E] = \Delta E_i \cap [E_{min}, E_{max}] .$$

Then with the pair production kernel of Eq. (3.4), the scattering kernels are unified as K,

$$K^{j\to i,\, n'\to n}(\vec{r}) = K_c{}^{j\to i,\, n'\to n}(\vec{r}) + K_{pp}{}^{j\to i,\, n'\to n}(\vec{r}).$$

And q^i in Eq. (3.2) is given

$$q^i(\vec{r}, \vec{\Omega}_n) = \sum_{j=1}^{i} \sum_{n'} \phi^j(\vec{r}, \vec{\Omega}_{n'}) K^{j\to i,\, n'\to n}(\vec{r}) + q_n{}^i(\vec{r}, \vec{\Omega}_n) + S^i(\vec{r}, \vec{\Omega}_n). \qquad (3.8)$$

When $S^i(\vec{r}, \vec{\Omega}_n)$ is given as a point source in case of one-dimensional sphere or two-dimensional cylinder, another kernel $K_o{}^{j\to i,\, n_o\to n}(\vec{r})$ is separately prepared. And uncollided scalar flux $\Psi_o{}^j(\vec{r})$ from the point source is multiplied to the K_o to obtain first collision source distribution.[1)]

3.4 Angular Flux Calculation

Equation (3.1) is solved for given source q^i in the same method as in neutron transport equation.[1] The q^i in Eq. (3.8) is separated into two components, that is,

$$q^i(\vec{r}, \vec{\Omega}_n) = SD^i(\vec{r}, \vec{\Omega}_n) + \sum_{n'} K^{i\to i,\, n'\to n}(\vec{r})\, \phi^i(\vec{r}, \vec{\Omega}_{n'}), \tag{3.9}$$

where SD^i is a fixed term for group i,

$$SD^i(\vec{r}, \vec{\Omega}_n) = \sum_{j=1}^{i-1} \sum_{n'} K^{j\to i,\, n'\to n}(\vec{r})\, \phi^j(\vec{r}, \vec{\Omega}_{n'}) + q_n{}^i(\vec{r}, \vec{\Omega}_n) + S^i(\vec{r}, \vec{\Omega}_n),$$

or, when S^i is given as a point source (for example, in cases of one-dimensional sphere and two-dimensional cylinder),

$$SD^i(\vec{r}, \vec{\Omega}_n) = \sum_{j=1}^{i-1} \sum_{n'} K^{j\to i,\, n'\to n}(\vec{r})\, \phi^j(\vec{r}, \vec{\Omega}_{n'}) + q_n{}^i(\vec{r}, \vec{\Omega}_n) + \sum_{j=1}^{i} K_o{}^{j\to i,\, n_o\to n}(\vec{r})\, \Psi_o{}^j(\vec{r}). \tag{3.10}$$

In the case of a point source, $\phi^i(\vec{r}, \vec{\Omega}_n)$ as the solution of Eq. (3.1) does not contain the uncollided component.

Angular flux $\phi^i(\vec{r}, \vec{\Omega}_n)$ is obtained with the combination of all the following methods:

(1) The direct integration method,
(2) Fine energy grid model,
(3) Order of sweep for $(\vec{r}, \vec{\Omega})$ mesh points in an iteration is completely same as in case of neutron calculation described in Sec. 3.6.1 in Ref. 1,
(4) Restart option for energy group continuation,
(5) Bootstrap option for spatial continuation in the z-direction and
(6) Coarse mesh rebalance of photon particles in each energy grid.

In case of gamma rays, an energy group is divided into 10 fine groups

called 'grids' having equal 'energy' width. The 10 grids in a group are numbered like ig=1,…,10 from the highest energy grid. There is no thermal energy group in case of gamma rays because the treated energy is down to not 0eV but 10keV, where no up-scattering exists. That is why all groups are able to be dealt with in the grid model.

When the number of times for iteration is fixed to 1, $\phi^{ig}(\vec{r}, \vec{\Omega}_{n'})$ in Eq.(3.9) is assumed to be equal to $\phi^{ig-1}(\vec{r}, \vec{\Omega}_{n'})$. The slowing down sources from (i-2)th and the upper groups are uniformly distributed into 10 grids in the group i. However, the slowing down sources from the 10 grids in the (i-1)th group and from the (ig-1) grids [jg=1,…,(ig-1)] in the i-th group are calculated very exactly with the scattering kernel $K^{jg \to ig, n' \to n}(\vec{r})$. These manners are all common to the case of neutron transport.[1)]

3.5 Benchmark Test of BERMUDA-2DG Code

In 1992, BERMUDA-2DG was tested comparing its calculational results with secondary gamma rays heating rates measured in an experiment[10] at the FNS facility[11] in JAERI. The heating rates were measured in an assembly of type 316L stainless steel, which was just the same as used in the neutron deep penetration experiment reported in Sec.4.1 of Ref.1.

The measured points in the assembly were also same, that is, 8, 28, 48, 68 and 88cm in depth along the axis of the cylindrical assembly. Omitting the details of measuring method (see Ref.10), we show only the results in the following:

Position (cm)	Nuclear heating rates (J/kg/source neutron)
8	$(7.06\pm0.837)\times10^{-18}$
28	$(7.49\pm0.0132)\times10^{-19}$
48	$(1.12\pm0.0215)\times10^{-19}$
68	$(2.19\pm0.0197)\times10^{-20}$
88	$(5.18\pm0.284)\times10^{-21}$

First, we performed a 121-group neutron transport calculation with the BERMUDA-2DN code, using the neutron library J449B.BERM125X.DATA (gr.5～125). During this procedure, we found that there was an error in the BERMUDA-2DN code in calculating the neutron slowing down source into the thermal group from the just upper group, that is, from 124th group to 125th group on the library.

Now, the neutron codes reported in Ref.1 have all been corrected for that error. But the C/E values of the BERMUDA-2DG results in Ref.10 were based on the neutron flux distribution obtained with the old version of the BERMUDA-2DN code, which contained the error.

A new neutron flux file have been prepared. Using this new file and the gamma rays group constants library J449B.BERM41G.DATA, a 41-group gamma rays transport calculation has been performed. The results are summarized with the C/E values, the C/E values[10] of old results and the C/E values[10] obtained with the DOT3.5 code.[12]

Position (cm)	Nuclear heating rates (J/kg/source neutron)		C/E Values		
	Measured	Calculated(new)	BERMUDA (new)	BERMUDA[10] (old)	DOT3.5[10]
8	7.06E-18[a]	8.002E-18	1.13	0.91	0.85
28	7.49E-19	8.995E-19	1.20	1.20	1.14
48	1.12E-19	1.564E-19	1.40	2.12	1.35
68	2.19E-20	2.861E-20	1.31	3.19	1.41
88	5.18E-21	4.454E-21	0.86	3.42	1.15

[a]Read as 7.06×10^{-18}

The DOT3.5 calculation referred above was also performed using a group constants library based on the nuclear data file JENDL-3.[5]

4. User's Manual

4.1 BERMUDA-1DG

4.1.1 JCL

The JCL (a set of job control languages) for the BERMUDA-1DG execution on the FACOM/VP2600 computer in JAERI is as follows:

(1) In case of gamma rays source only (without neutron-induced secondary gamma rays source)

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
       T.05 W.01 C.00 I.02 E.01 SRP
       OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),CLASS=0,NOTIFY=Jxxxx
       OPTP PASSWORD=xxxxxxxx
//    EXEC LMGO,LM=J9091.BERMUDA,PNM=BERMD1DG(*1)
//FT01F001 DD DISP=SHR,DSN=Jxxxx.FLUX1DG.DATA(*2)
//FT03F001 DD DISP=SHR,DSN=Jxxxx.SDB1DG.DATA(*3)
//FT04F001 DD DISP=SHR,DSN=J449B.BERM41G.DATA,LABEL=(,,,IN)
//SYSIN    DD DISP=SHR,DSN=Jxxxx.DATA1DG.DATA(*4)
//FT08F001 DD DUMMY(*5)
++
//
```

(2) In case of using a neutron flux file for calculating secondary gamma rays source in BERMUDA-1DG

The one line of the JCL(*5) in the above JCL (1) is substituted with the next one to use a neutron flux file from BERMUDA-1DN.

```
//FT08F001 DD DISP=SHR,DSN=Jxxxx.FLUX1DN.DATA
```

(3) In case of executing both BERMUDA-1DN[1] and BERMUDA-1DG in a job.

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.06 W.03 C.00 I.04 E.01 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),CLASS=0,NOTIFY=Jxxxx
      OPTP PASSWORD=xxxxxxxx
//    EXEC LMGO,LM=J9091.BERMUDA,PNM=BERMD1DN
//FT01F001 DD UNIT=TSSWK,SPACE=(TRK,(70,10)),DSN=Jxxxx.FLUX1DN.DATA,
//    DISP=(NEW,PASS),DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
//FT02F001 DD UNIT=WK10,SPACE=(TRK,(100,50)),DISP=(NEW,DELETE,DELETE),
//    DSN=&&WORK,DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
//FT03F001 DD DUMMY
//FT04F001 DD DISP=SHR,DSN=J449B.BERM125X.DATA,LABEL=(,,,IN)
//SYSIN    DD DISP=SHR,DSN=Jxxxx.DATA1DN.DATA
//    EXEC LMGO,LM=J9091.BERMUDA,PNM=BERMD1DG
//FT01F001 DD DISP=SHR,DSN=Jxxxx.FLUX1DG.DATA
//FT03F001 DD DUMMY
//FT04F001 DD DISP=SHR,DSN=J449B.BERM41G.DATA,LABEL=(,,,IN)
//SYSIN    DD DISP=SHR,DSN=Jxxxx.DATA1DG.DATA
//FT08F001 DD DISP=OLD,DSN=Jxxxx.FLUX1DN.DATA
++
//
```

($1) There has already been a load module J9091.BERMUDA.LOAD(BERMD1DG) prepared for a public use in JAERI.

If necessary, a new load module is able to be created on a disk from the source module J9091.BERMUDA.FORT77(BERMD1DG). The JCL for creating a new load module is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
```

```
      T.01 W.01 C.02 I.02 E.00 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),NOTIFY=Jxxxx,PASSWORD=xxxxxxxx
//    EXEC FORT77VE,SO=J9091.BERMUDA,
//     A='ELM(BERMD1DG),SOURCE,NOVMSG,NOVSOURCE',LCT=62
//    EXEC LKEDCT77,LM=Jxxxx.BERMD1DG,UNIT=xxxxx,MODS='07,07,1',A=MAP
++
//
```

These steps of compilation and linkage are executed rather rapidly on the FACOM/M780 scalar computer. The new load module is applied by replacing the above "LM=J9091.BERMUDA,PNM=BERMD1DG," (*1) with "LM=Jxxxx.BERMD1DG".

(*2) The gamma rays flux file Jxxxx.FLUX1DG.DATA has to be allocated beforehand as:

```
//FT01F001 DD UNIT=xxxxx,SPACE=(TRK,(30,10)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLUX1DG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the spatial distributions of angular and scalar flux etc. of gamma rays for all of the calculated energy groups. It can be used for editing the output results.

(*3) The grid source file Jxxxx.SDB1DG.DATA has to be allocated beforehand as:

```
//FT03F001 DD UNIT=xxxxx,SPACE=(TRK,(10,05)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.SDB1DG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file is necessary for restarting the job, and can be deleted after the calculation up to the last (IMAX-th) energy group has been completed.

Usually a one-dimensional problem is rapidly completed in a batch job. So, when required CPU time for the job is sufficient for completing calculation up to the last group, the one line of the JCL(*3) may be substituted with

```
//FT03F001 DD DUMMY
```

without allocating the Jxxxx.SDB1DG.DATA.

($4) The input data file Jxxxx.DATA1DG.DATA has to be allocated beforehand as:

```
//FT05F001 DD UNIT=xxxxx,SPACE=(TRK,(01,01)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.DATA1DG.DATA,
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120,DSORG=PS)
```

The content of this file is described in Sec.4.1.2. Otherwise, the one line of the JCL($4) is substituted with

```
//SYSIN    DD *
      [input data described in Sec.4.1.2]
/*
```

without allocating the Jxxxx.DATA1DG.DATA.

4.1.2 Input Data

#01 (F6.0) 1 line

・TMAX(≡300.) : CPU time (sec) to terminate the job and to prepare the disk files for restarting the next job

#02 (I3) 1 line

・KIND(≡0) : dummy

#03 (2I3) 1 line

・IRSTRT(≡1) : group no. to be restarted (initially ≡1)

・ITMAX : maximum number of iteration times for each energy grid (ITMAX＝1, 2 or 3)
(ITMAX is defined as 1, if 0 or blank is input.)

#04 (18A4) 1 line

・Problem title : any characters, numbers or blanks describing the problem on columns 1～72

#05 (8I6, 2E12.5) 1 line

・IMAX : total number of energy groups for this problem (≦41)

・IP : geometry

$$IP = \begin{cases} 0 \cdots \text{slab (infinite in x- and y-directions)} \\ \\ 2 \cdots \text{sphere} \end{cases}$$

・MMAX : number of kinds of mixture (≦20)

・KMAX : number of spatial regions (MMAX≦KMAX≦20)
(In a region, mixture is assigned to be homogeneous and mesh sizes (Δz or Δr) are assigned to be equal to each other.)

・I1LIB : group no. "on the group constants library" where the group 1 is to be defined
(for example, IMAX+I1LIB≦42 for J449B.BERM41G.DATA)

In BERMUDA, the I1LIB-th group on the library is called as "group 1".

・NILIB : initial group no. of the FT08 neutron flux file "on the neutron

group constants library" (NILIB＝0 if FT08 is dummy.)

・NFLIB : final group no. of the FT08 neutron flux file "on the neutron group constants library" (NFLIB＝0 if FT08 is dummy.)
1≦NILIB≦NFLIB≦NMAXL and NFLIB-NILIB+1＝IMAXN (Sec.3.1)

・IPS : type of the fixed source

$$IPS=\begin{cases} -1 \cdots \text{secondary gamma rays source only} \\ 0 \cdots \text{spatially distributed source} \\ 1 \cdots \text{point source (only at the center of the sphere)} \end{cases}$$

・ER : upper energy (eV) for the group I of the problem
EUP(I1LIB+1)＜ER≦EUP(I1LIB)

・EPS : convergence criterion (for angular flux) to be used to terminate the grid iteration before ITMAX (usually 10^{-3})

#06 (2013) 1 line

・(MM(MK),MK＝1,MMAX) : number of nuclides to be included in each mixture
(1≦MM(MK)≦10)
(For a vacuum, assign one dummy nuclide which is contained in another mixture. Input its code number in #12 and atomic number density (0.) in #13.)

#07 (1016) [(KMAX+9)/10] lines

The brackets [⋯] means the integer discarding the fractions.

・(MR(K),K＝1,KMAX) : mixture no. (≡MK defined in #6) to be assigned to each region

#08 (1016) [(KMAX+9)/10] lines

・(INTER(K),K＝1,KMAX) : number of mesh intervals between the 'origin' and the outer boundary of each region (even number only)
(2≦INTER(1)＜INTER(2)＜⋯＜INTER(KMAX)≦260-KMAX)

#09 (10F6.3) [(KMAX+9)/10] lines

・(DR(K),K＝1,KMAX) : mesh size Δz or Δr (cm) for each region (not the region thickness)

#10 (6E12.5) 2 lines

・(BCR(L), L＝11, 20) : right (outer) boundary condition (10 words)

$$BCR(L) \equiv \begin{cases} -1. \cdots \text{symmetry condition (only for IP＝0)} \\ 0. \cdots \text{vacuum boundary condition (for IP＝0 and 2)} \end{cases}$$

(at the present, group independent only)

#11 (6E12.5) 2 lines when IP＝0, not necessary when IP＝2

・(BCL(L), L＝1, 10) : left (origin) boundary condition for slab (10 words)

$$BCL(L) \equiv \begin{cases} -1. \cdots \text{symmetry condition} \\ 0. \cdots \text{vacuum boundary condition} \end{cases}$$

(at the present, group independent only)

#12 (10I6) MMAX lines

・(MCODE(M, MK), M＝1, MM(MK)) : code no. of each nuclide in the mixture MK defined in the group constants library to be used (for example, see Sec. 2.1)

(The order of nuclides in a mixture is able to be arbitrary.)

Repeat this in the order of MK＝1, …, MMAX renewing the line for each mixture.

#13 (6E12.5) [{MM(MK)+5}/6] lines for each mixture

・(AN(M, MK), M＝1, MM(MK)) : effective number density ($10^{24}cm^{-3}$) of each nuclide in the mixture MK

(The order of nuclides in a mixture must be the same as in #12.)

Repeat this in the order of MK＝1, …, MMAX renewing the line for each mixture.

When IPS＝-1 in #5, data of #14～#19 are not necessary to be input.

#14 (2I6) 1 line

・N1 : the first mesh point no. to give spatial distribution of non-zero independent source in #15

・N2 : the last mesh point no. to give spatial distribution of non-zero independent source in #15

If IPS＝1 in #5 then N1＝N2＝1. Otherwise, 1≦N1＜N2≦NMAX.
(NMAX: see (3) below)

In BERMUDA, the numbering of the mesh points is as follows:

(1) "1" for the origin,

(2) doubly (twice) numbered as "INTER(K)+K" and "INTER(K)+K+1" for the interface between the K-th and the (K+1)-th regions where K＝1,…,KMAX-1 (for treating spatial discontinuity of the macroscopic cross sections and the source distribution at the interfaces) and

(3) "NMAX＝INTER(KMAX)+KMAX" (≦260) for the outermost mesh point.

#15 (6E12.5)　　{[(N2-N1)/6]+1} lines

・(S1(N), N＝N1, N2) : spatial distribution of independent source
Independent source is given in the form of a function with separation of variables as S1(N)×S2(I)×S3(L).
(Each of the S1, S2 and S3 should be normalized to its correct magnitude, respectively. However, it is also valid that the product of the S1, S2 and S3 has the correct normalized value for each energy group(*).)

#16 (2I6)　　1 line

・I1 : the first energy group no. to give energy spectra of non-zero independent source in #17 (see Sec.2.2, but note that the group no. is defined so that the I1LIB-th group in Sec.2.2 is group 1.)

・I2 : the last energy group no. to give energy spectra of non-zero independent source in #17
If the source is of mono-energy (monochromatic), I1＝I2＝1.
Otherwise, 1≦I1＜I2≦IMAX.

#17 (6E12.5)　　{[(I2-I1)/6]+1} lines

・(S2(I), I＝I1, I2) : energy spectra of independent source
(As BERMUDA has been programmed not in a continuous energy model but in a usual multigroup model, only the S2 (except the S1 and S3) must be given as integrated value for group i over ΔE_i.)
The S2(I) is generally normalized to be 1 integrated over energy, that is,

$$\sum_{I=I1}^{I2} S2(I) = 1.$$

(However, note the proviso(*) under #15.)

#18 (2I6) 1 line

・L1 : the first ordinate no. to give angular distribution of non-zero independent source in #19

・L2 : the last ordinate no. to give angular distribution of non-zero independent source in #19

If the source is mono-directional, L1＝L2.

Otherwise, $1 \leqq L1 < L2 \leqq 20$.

#19 (6E12.5) {[(L2-L1)/6]+1} lines

・(S3(L), L＝L1, L2) : angular distribution of independent source

The S3(L) is generally normalized to be 1 integrated over the unit sphere, that is,

$$2\pi \sum_{L=L1}^{L2} W_L S3(L) = 1.$$ (W_L : weight for Gaussian quadrature of order 20)

(However, note the proviso(*) under #15.)

Some examples of input data for the BERMUDA-1DG code are shown in Figs.4.1 and 4.2.

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8

 60.                                                                          #01
  0                                                                           #02
  1                                                                           #03
     WATER 10MEV , POINT ISOTROPIC , 07/23/84 MON.                            #04
    40      2      1      6      2      0      0      1 1.0002    +7 1.0       -3 #05
  2                                                                           #06
     1      1      1      1      1      1                                     #07
     4     14     22     36     56    114                                     #08
2.71533.37845.63069.652911.26127.182                                         #09
 0.            0.            0.            0.            0.            0.     #10
 0.            0.            0.            0.                                  "
   117    807                                                                #12
 6.691     -2 3.346     -2                                                    #13
     1      1                                                                 #14
 1.                                                                           #15
     1      1                                                                 #16
 1.                                                                           #17
     1     20                                                                 #18
 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2      #19
 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2       "
 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2 7.957747 -2       "
 7.957747 -2 7.957747 -2                                                       "
```

Fig.4.1 Example of input data for BERMUDA-1DG (IPS=1)

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8

 60.                                                                          #01
  0                                                                           #02
  1                                                                           #03
     ONE DIMENSIONAL GAMMA-RAY TRANSPORT PROGRAM : BERMUDA-1DG                #04
    41      2      4      4      1      5    125     -1 1.4       +7 1.0       -3 #05
  4  6  5  4                                                                  #06
     1      2      3      4                                                   #07
    20     44     66     82                                                   #08
0.5  1.0058.96136.91938                                                       #09
 0.            0.            0.            0.            0.            0.     #10
 0.            0.            0.            0.                                  "
  2407   2607   2807   2507                                                  #12
   307    317   2407   2607   2807   2507                                     "
   607   2407   2607   2807   2507                                            "
  2407   2607   2807   2507                                                  "
 1.751     -3 6.349     -3 7.303     -4 8.185     -5                          #13
 2.507     -3 3.128     -2 3.086     -3 1.075     -2 1.374     -3 2.023     -4  "
 6.930     -2 1.751     -3 6.349     -3 7.303     -4 8.185     -5              "
 1.161     -3 4.159     -3 4.821     -4 5.632     -5                          "
```

Fig.4.2 Example of input data for BERMUDA-1DG (IPS=-1)

4.1.3 Output Data

The output data of BERMUDA-1DG are stored on the magnetic disk FT01 (Jxxxx.FLUX1DG.DATA; see Sec.4.1.1 (S2)) and are also given on the printer.

The data on the output disk are as follows:

(1) In case of IPS≠1, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

((PSI(N,L),N＝1,260),L＝1,20),(TPSI(N),N＝1,260),

where PSI(N,L) : $\phi^i(r_N, \omega_L)$ and

TPSI(N) : $\Psi^i(r_N) = 2\pi \sum_{L=1}^{20} W_L \phi^i(r_N, \omega_L)$.

(2) In case of IPS＝1, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

((PSI(N,L),N＝1,260),L＝1,20),(TPSI(N),N＝1,260),
(PSI0(N),N＝1,260),(PSI00(L),L＝1,20),

where PSI(N,L) : $\phi^i(r_N, \omega_L)$ (without component of uncollided flux),

TPSI(N) : $\Psi^i(r_N) = 2\pi \sum_{L=1}^{20} W_L \phi^i(r_N, \omega_L) + \Psi_0^i(r_N)$,

PSI0(N) : $\Psi_0^i(r_N)$ (uncollided flux) and
PSI00(L) : $S^i(0, \omega_L)$ (point source at the origin).

The data on the output print are as follows:

(a) list of input file Jxxxx.DATA1DG.DATA (see Sec.4.1.1 (S4)) like Figs.4.1 or 4.2,
(b) list of the main input parameters with explanatory captions,

(The items (c)～(f) below are repeated for each energy group i (i＝1, …, IMAX).)

(c) CPU+VU time (sec) accumulated from the start of computation (EXEC LMGO) until the end of each main calculational item,

(d) when the convergence has been attained or ITMAX iterations have been finished for the 10-th grid,

・photon balance parameters; F, GAIN, ABBS, SELF, XLEK (see Sec. 3.7 of Ref.1) integrated over the entire spatial region dealing with it as a single coarse mesh region,

・group no. i, iteration times IT, residual VERGF,

where $VERGF = \max_{N,L} \left| \{\phi^{ig(IT-1)}(r_N, \omega_L)/\phi^{ig(IT)}(r_N, \omega_L)\} - 1 \right| < \varepsilon$

(N, L : except the cases where $\phi^{ig(IT)}(r_N, \omega_L) = 0$),

IT : iteration times (IT＝1, 2, …),

(As the energy grid model is used for all groups, these printed photon balance parameters and VERGF are meaningless, because the iteration is terminated by ITMAX (≦3) times. In addition, these parameters are obtained only from the data of the last (10th) grid in the group i.)

(e) ・the upper energy boundary EUP(i) (eV),

・the lower energy boundary EUP(i+1) (eV),

・the energy width ΔE_i (eV),

(f) gamma rays scalar flux $\Psi^i(r_N)$ for N＝1, …, NMAX and

(g) spatial distribution of dose rate (Sv/hr)

$$\sum_{i=1}^{IMAX} DCONV(i)\Psi^i(r_N) \quad \text{for } N=1, \cdots, NMAX,$$

where DCONV is a conversion factors installed in BERMUDA-1DG.

The STOP code 2222 indicates that the input fixed source for the group 1 is zero including the secondary gamma rays source.

4.2 BERMUDA-2DG

4.2.1 JCL

The JCL for the BERMUDA-2DG execution on the FACOM/VP2600 computer in JAERI is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.10 W.03 C.00 I.09 E.04 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),CLASS=7,NOTIFY=Jxxxx (*1)
      OPTP PASSWORD=xxxxxxxx
//    EXEC LMGO,LM=J9091.BERMUDA,PNM=BERMD2DG,A='HIO=(01,09)' (*2)
//FT01F001 DD DISP=SHR,DSN=Jxxxx.FLX701.DATA (*3)
//FT02F001 DD DISP=SHR,DSN=Jxxxx.BOUNDFXG.DATA (*4)
//FT03F001 DD UNIT=WK10,SPACE=(TRK,(100,50)),DISP=(NEW,DELETE,DELETE),
//     DSN=&&WORK,DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
//FT04F001 DD DISP=SHR,DSN=J449B.BERM41G.DATA,LABEL=(,,,IN)
//SYSIN    DD DISP=SHR,DSN=Jxxxx.DATA2DG.DATA (*5)
//FT08F001 DD DISP=SHR,DSN=Jxxxx.FLUX2DN.DATA (*6)
//FT09F001 DD DISP=SHR,DSN=Jxxxx.FLX709.DATA (*7)
//FT10F001 DD DISP=SHR,DSN=Jxxxx.FLUX2DG.DATA (*8)
//FT11F001 DD DISP=SHR,DSN=Jxxxx.SDB2DG.DATA (*9)
++
//
```

(*1) "CLASS=7" is a night job for free submission. Beside this, there are the classes 6 and 8 which need an approval of the Computing and Information Systems Center of JAERI for submission, and of which the class 8 is a night job. For these classes, permitted CPU time (T.xx), print lines (W.xx) and I/O times (EXCP I.xx) have different values from those of the class 7.

(*2) There has already been a load module J9091.BERMUDA.LOAD(BERMD2DG) prepared for a public use in JAERI.

If necessary, a new load module is able to be created on a disk from the source module J9091.BERMUDA.FORT77(BERMD2DG). The JCL for creating a new load module is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.02 W.03 C.02 I.02 E.00 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),NOTIFY=Jxxxx,PASSWORD=xxxxxxxx
//    EXEC FORT77VE,SO=J9091.BERMUDA,
//     A='ELM(BERMD2DG),SOURCE,NOVMSG,NOVSOURCE',LCT=62
//    EXEC LKEDCT77,LM=Jxxxx.BERMD2DG,UNIT=xxxxx,MODS='10,10,1',A=MAP
++
//
```

These steps of compilation and linkage are executed rather rapidly on the FACOM/M780 scalar computer. The new load module is applied by replacing the above "LM=J9091.BERMUDA,PNM=BERMD2DG" (\$2) with "LM=Jxxxx.BERMD2DG".

(\$3) The HIO (high-speed input/output) work file for the angular and scalar fluxes Jxxxx.FLX701.DATA has to be allocated beforehand as:

```
//FT01F001 DD UNIT=TSSWK,SPACE=(CYL,082,,CONTIG),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLX701.DATA,
//     DCB=(RECFM=F,LRECL=23000,BLKSIZE=23000,DSORG=PS)
```

This file contains the spatial distributions of the angular and scalar photon fluxes for all of the calculated energy groups as a HIO work file for calculating the slowing down source from the upper energy groups.

So, this file can be deleted after the job has been successfully terminated in TMAX sec (see Sec.4.2.2) because the same data are stored in the FT10 (Jxxxx.FLUX2DG.DATA(\$8)) for restarting the job. The main purpose of the FT01(\$3) and FT09(\$7) is to utilize the HIO option for saving the I/O times (EXCP). In fact, the TSSWK is automatically deleted at 8:00 a.m. (the TSSWK2 at 5:00 p.m.) in JAERI. The HIO option needs to allocate the file

'contiguously' on the disk (CONTIG), and the FT01 and FT09 need to be allocated every time (or every day) before submitting the restarting job.

At the present, the specifications of the disk in JAERI are as follows:

1 VOL = 1,326 CYL × 2 (= 19,890 TRK × 2),

1 CYL = 15 TRK and

1 TRK = 47,476 bytes.

However, BLKSIZE cannot exceeds 32,767 bytes.

($4) The boundary flux file Jxxxx.BOUNDFXG.DATA has to be allocated beforehand as:

```
//FT02F001 DD UNIT=xxxxx,SPACE=(TRK,(10,05)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.BOUNDFXG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the boundary flux in case of the bootstrap option (see Sec.3.6.2 in Ref.1). In the first step, the boundary flux is written in this file; and in the second step, the boundary flux is supplied from the file. When the bootstrap option is not used (ISTEP＝0 in Sec.4.2.2), the one line of the JCL($4) is not necessary as well as allocation of the file.

($5) The input data file Jxxxx.DATA2DG.DATA has to be allocated beforehand as:

```
//FT05F001 DD UNIT=xxxxx,SPACE=(TRK,(01,01)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.DATA2DG.DATA,
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120,DSORG=PS)
```

The content of this file is described in Sec.4.2.2. Otherwise, the one line of the JCL($5) is substituted with

```
//SYSIN    DD *
     [input data described in Sec.4.2.2]
/*
```

without allocating the Jxxxx.DATA2DG.DATA.

($6) The neutron flux file Jxxxx.FLUX2DN.DATA is an output file of BERMUDA-2DN. If the problem does not need the secondary gamma rays source, the one line of the JCL($6) is substituted with the next one.

```
//FT08F001 DD DUMMY
```

($7) The HIO work file for the uncollided flux has to be allocated beforehand as:

```
//FT09F001 DD UNIT=TSSWK,SPACE=(CYL,03,,CONTIG),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLX709.DATA,
//     DCB=(RECFM=F,LRECL=23000,BLKSIZE=23000,DSORG=PS)
```

This file contains the spatial distribution of the uncollided gamma rays flux for all of the calculated energy groups as a HIO work file for calculating the first collision source from the self and the upper groups in Eq.(3.10).

This file can also be deleted after the job has been successfully terminated in TMAX sec same as the FT01, because the same data are stored in the FT10 for restarting the job.

If IPS=0, the one line of the JCL($7) is not necessary as well as allocation of the file.

($8) The gamma rays flux file Jxxxx.FLUX2DG.DATA has to be allocated beforehand as:

```
//FT10F001 DD UNIT=xxxxx,SPACE=(TRK,(1200,50)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLUX2DG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the spatial distributions of angular and scalar flux etc. of gamma rays for all of the calculated energy groups. It is used for restarting the job for energy group continuation and also can be used for editing the output results.

Note that the contents of the Jxxxx.FLUX2DG.DATA for the bootstrap step 1 vanish when the same file is used in the step 2. If it is necessary to save the data obtained in the step 1, dual files have to be allocated as Jxxxx.FLUX2DG1.DATA and Jxxxx.FLUX2DG2.DATA for each step.

($9) The grid source file Jxxxx.SBD2DG.DATA has to be allocated beforehand as:

```
//FT11F001 DD UNIT=xxxxx,SPACE=(TRK,(280,20)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.SDB2DG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file is necessary for restarting the job as well as the FT10, and can be deleted after the calculation up to the IMAX-th group has been completed (in case of ISTEP≠0, up to the IMAX-th group in the step 2).
The contents of the FT11 are:

(1) the group no. i_R (Up to the i_R group the calculation has been completed.) and
(2) the grid source into the ten grids within the group i_R+1 from the groups 1 ～ i_R-1 and from the ten grids within the group i_R.

4.2.2 Input Data

#01 (F6.0) 1 line

・TMAX : CPU time (sec) to terminate the job and to prepare the disk files for restarting the next job (If CLASS＝7, then TMAX＝7000.)

#02 (4I3) 1 line

・IRSTRT : group no. to be restarted (initially ≡1)

・ISTEP : step no. for bootstrap option

$$ISTEP=\begin{cases}0 \cdots \text{no bootstrap option}\\ 1 \cdots \text{the first step}\\ 2 \cdots \text{the second step}\end{cases}$$

・IFACE : interface z-mesh point no. for bootstrap option (0 when ISTEP＝0) IFACE must be on the bottom boundary mesh point of a partition in the z-direction. (The numbering method for mesh points is described in #10.)
When ISTEP＝2, IFACE has a different value from that in ISTEP＝1.

・ITMAX : maximum number of iteration times for each energy grid (ITMAX＝1, 2 or 3)
(ITMAX is defined as 1, if 0 or blank is input.)

#03 (18A4) 1 line

・Problem title : any characters, numbers or blanks describing the problem on columns 1～72

#04 (11I4, 2E12.5) 1 line

・IMAX : total number of energy groups for this problem (≦41)

・MMAX : number of mixtures (≦20)

・KMAX : number of spatial regions (MMAX≦KMAX)
Definition of a 'region' is that it is a rectangular part on the (r, z) plane, where mixture is assigned to be homogeneous.
The (r, z) plane must be completely covered with the KMAX regions.
Actually a 'region' is a ring-shaped volume made by rotating the rectangular around the axis of the cylinder (z＝0).

・I1LIB : group no. "on the group constants library" where the group 1 of this problem is to be defined

(for example, IMAX+I1LIB≦42 for J449B.BERM41G.DATA)

In BERMUDA, the I1LIB-th group on the library is called as "group 1".

・NILIB : initial group no. of the FT08 neutron flux file "on the neutron group constants library" (NILIB＝0 if FT08 is dummy.)

・NFLIB : final group no. of the FT08 neutron flux file "on the neutron group constants library" (NFLIB＝0 if FT08 is dummy.)
1≦NILIB≦NFLIB≦NMAXL and NFLIB-NILIB+1＝IMAXN (Sec.3.1)

・IPS : type of the fixed source

$$IPS = \begin{cases} -1 \cdots \text{secondary gamma rays source only} \\ 0 \cdots \text{spatially distributed source} \\ IZPS \cdots \text{point source on the z-axis of the cylinder} \\ \quad (IZPS \geqq 1) \end{cases}$$

The IZPS is the z-mesh point no. for the point source. When IZPS＝1, z(IZPS)＝0 (origin). The numbering method for the mesh points is described in #10. The point source cannot be placed on an interface between partitions in the z-direction.

・NRR : number of partitions in the r-direction (NRR≦20)
In each partition, mesh sizes (Δr) are assigned to be equal to each other.

・NRZ : number of partitions in the z-direction (NRZ≦20)
In each partition, mesh sizes (Δz) are assigned to be equal to each other.

・NEWCF : input of new conversion factors

$$NEWCF = \begin{cases} 0 \cdots \text{conversion factors prepared in the code are used.} \\ 1 \cdots \text{new conversion factors or responses are input in} \\ \quad \text{the items \#20, 21 below and used.} \end{cases}$$

・IPSN : type of the fixed source for calculation of the FT08 neutron flux file

$$IPSN = \begin{cases} 0 \cdots \text{spatially distributed neutron source} \\ 1 \cdots \text{point neutron source} \end{cases}$$

・ER : upper energy (eV) for the group 1 of the problem
EUP(I1LIB+1)＜ER≦EUP(I1LIB)

・EPS : convergence criterion (for angular flux) to be used to terminate

the grid iteration before ITMAX (usually 10^{-3})

#05 (2013) 1 line

・(MM(MK), MK = 1, MMAX) : number of nuclides to be included in each mixture
($1 \leqq MM(MK) \leqq 10$)
(For a vacuum, assign one dummy nuclide which is contained in another mixture. Input its code number in #12 and atomic number density (0.) in #13.)

#06 (10I6) [(NRR+9)/10] lines

The brackets [⋯] means the integer discarding the fractions.

・(INTERR(KR), KR = 1, NRR) : number of mesh intervals between the origin and the outer boundary of each partition in the r-direction
(Either even or odd numbers are valid.)
($1 \leqq INTERR(1) < INTERR(2) < \cdots < INTERR(NRR) \leqq 60-NRR$)

#07 (10F6.3) [(NRR+9)/10] lines

・(DRR(KR), KR = 1, NRR) : mesh size Δr (cm) for each partition in the r-direction
(not the partition thickness)

#08 (10I6) [(NRZ+9)/10] lines

・(INTERZ(KZ), KZ = 1, NRZ) : number of mesh intervals between the origin and the top boundary of each partition in the z-direction
(Either even or odd numbers are valid.)
($1 \leqq INTERZ(1) < INTERZ(2) < \cdots < INTERZ(NRZ) \leqq 110-NRZ$)

#09 (10F6.3) [(NRZ+9)/10] lines

・(DZZ(KZ), KZ = 1, NRZ) : mesh size Δz (cm) for each partition in the z-direction
(not the partition thickness)

#10 (5I6) KMAX lines

・(J1(K), J2(K), I1(K), I2(K), MR(K), K = 1, KMAX) : assignment of composition
J1(K) : left mesh point no. of the region K

J2(K) : right mesh point no. of the region K
I1(K) : bottom mesh point no. of the region K
I2(K) : top mesh point no. of the region K
MR(K) : mixture no. for the region K (≡MK defined in #5)
(1≦J1<J2≦NRMAX≦60 and 1≦I1<I2≦NZMAX≦110)

In BERMUDA, the numbering of the mesh points is as follows:
(1) "1" for the origin,
(2) doubly (twice) numbered as "INTERR(KR)+KR" and "INTERR(KR)+KR+1" for the interface between the KR-th and the (KR+1)-th partitions in the r-direction where KR=1,…,NRR-1 (for treating spatial discontinuity of the macroscopic cross sections and the source distribution at the interfaces) and
(3) "NRMAX=INTERR(NRR)+NRR" ≦60 for the outermost mesh point in the r-direction.
And it is same for the z-direction except "NZMAX=INTERZ(NRZ)+NRZ" ≦110.

#11 (2F6.3) 1 line
・BCTOP : top boundary condition for z=z(NZMAX)
・BCBOT : bottom boundary condition for z=0.

boundary conditions≡
-1. … symmetry condition
0. … vacuum boundary condition

#12 (10I6) MMAX lines
・(MCODE(M,MK),M=1,MM(MK)) : code no. of each nuclide in the mixture MK defined in the group constants library to be used (see Sec.2.1)
(The order of nuclides in a mixture is able to be arbitrary.)
Repeat this in the order of MK=1,…,MMAX renewing the line for each mixture.

#13 (6E12.5) [(MM(MK)+5)/6] lines for each mixture
・(AN(M,MK),M=1,MM(MK)) : effective number density ($10^{24}cm^{-3}$) of each nuclide in the mixture MK
(The order of nuclides in a mixture must be same as in #12.)
Repeat this in the order of MK=1,…,MMAX renewing the line for each

mixture.

When IPS=-1 in #04, data of #14～#19 below are not necessary to be input.

#14 (4I6) 1 line

- IZ1 : the first mesh point no. to give axial distribution of non-zero independent source in #15
- IZ2 : the last mesh point no. to give axial distribution of non-zero independent source in #15
- JR1 : the first mesh point no. to give radial distribution of non-zero independent source in #15
- JR2 : the last mesh point no. to give radial distribution of non-zero independent source in #15

  These mesh points must be given in the definition of (1)～(3) in #10 ($1 \leqq IZ1 \leqq IZ2 \leqq NZMAX$ and $1 \leqq JR1 \leqq JR2 \leqq NRMAX$). When IPS=0 in #04, S1 in #15 is a volume source ($IZ1 < IZ2$ and $JR1 < JR2$). When $IPS \geqq 1$, S1 is a point source ($IZ1 = IZ2 = IPS$ and $JR1 = JR2 = 1$).

#15 (6E12.5) {[(JR2-JR1)/6]+1} lines

- (S1(JR, IZ), JR=JR1, JR2) : spatial distribution of independent source

  Independent source is given in the form of a function with separation of variables as $S1(JR, IZ) \times S2(I) \times S3(L)$.

  (Each of the S1, S2 and S3 should be normalized to its correct magnitude, respectively. However, it is also valid that the product of the S1, S2 and S3 has the correct normalized value for each energy group(*).)

Repeat this in the order of IZ=IZ1, …, IZ2.

#16 (2I6) 1 line

- I1 : the first energy group no. to give energy spectre of non-zero independent source in #17 (see Sec. 2.2, but note that the group no. is defined so that the I1LIB-th group in Sec. 2.2 is group 1.)
- I2 : the last energy group no. to give energy spectre of non-zero independent source in #17

  If the source is of mono-energy (monochromatic), I1=I2=1.

  Otherwise, $1 \leqq I1 < I2 \leqq IMAX$.

#17 (6E12.5) {[(I2-I1)/6]+1} lines

・(S2(I), I=I1, I2) : energy spectre of independent source

(As BERMUDA has been programmed not in a continuous energy model but in a usual multigroup model, only the S2 (except the S1 and S3) must be given as integrated value for group i over ΔE_i.)

The S2(I) is generally normalized to be 1 integrated over energy, that is,

$$\sum_{I=I1}^{I2} S2(I) = 1.$$

(However, note the proviso(*) under #15.)

#18 (2I6) 1 line

・L1 : the first ordinate no. to give angular distribution of non-zero independent source in #19 (see Fig.3.3 in Ref.1)

・L2 : the last ordinate no. to give angular distribution of non-zero independent source in #19

If the source is mono-directional, L1=L2.

Otherwise, $1 \leqq L1 < L2 \leqq 40$. (S3(L) for L=41,…,48 are assumed to have equal values to the adjacent (just right) ordinates, respectively.)

#19 (6E12.5) {[(L2-L1)/6]+1} lines

・(S3(L), L=L1, L2) : angular distribution of independent source

The S3(L) is generally normalized to be 1 integrated over the unit sphere, that is,

$$\sum_{L=L1}^{L2} \Delta \vec{\Omega}_L S3(L) = 1.$$

(However, note the proviso(*) under #15.)

When NEWCF=0 in #04, data of #20 and #21 below are not necessary to be input.

#20 (18A4) 1 line

・Response name : any characters, numbers or blanks describing the conver-

sion factors given in #21 on columns 1～72

#21 (8F8.4)　　{[(NGMAX+7)/8]+1} lines

・(CF(I), I＝1, NGMAX) : conversion factors for 'all library groups'

An example of input data for the BERMUDA-2DG code is shown in Fig. 4.3.

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8

2650.                                                                          #01
 1  0  0  1                                                                   #02
SUS316 ASSEMBLY NUCLEAR HEATING 19/09/90 WED.                                  #03
 41   4  13   1   5 125   1   8   6   1   1 1.4      +7 5.0      -3           #04
 2 10  7  9                                                                    #05
    6     7     8    10    11    36    37    42                               #06
3.75  0.8   2.5   4.6   0.8   8.488 2.0   12.0                                #07
   16    17    27    28    48    68                                           #08
15.5  2.0   7.8   1.6   3.0   3.0                                            #09
    1    42     1    17     1    REG 1 AIR FRONT PART                        #10
   43    44     1    17     2    REG 2 MORTAR                                 "
   45    50     1    19     3    REG 3 ROOM WALL                              "
    1    14    18    30     1    REG 1-2 AIR FRONT PART                       "
   15    16    18    32     4    REG 4 FE TEST PORT FLAME                     "
   17    44    18    19     2    REG 2-2 MORTAR                               "
   17    50    20    32     3    REG 3-2 ROOM WALL                            "
    1     7    31    32     1    REG 1-3 AIR FRONT PART                       "
    8    14    31    32     4    REG 4-2 FE TEST PORT FLAME                   "
    1     9    33    53     4    REG 4-3 FE TEST PORT SUS316                  "
   10    50    33    53     3    REG 3-3 ROOM WALL                            "
    1    11    54    74     4    REG 4-4 FE TEST PORT SUS316                  "
   12    50    54    74     3    REG 3-4 ROOM WALL                            "
0.   -1.                                                                       #11
  707   807                                                                    #12
  117   807   807  1307  1307  1307  1407  1407  1407  2607                   "
  807   117  1307  1307  1307  1407  2607                                     "
  607  1407  1407  1407  2407  2507  2607  2807  4207                         "
4.2000   -5 1.1300   -5                                                       #13
9.4246   -3 7.4297   -4 3.7680   -2 5.0802   -4 4.6874   -4 1.9408   -3      "
1.1347   -2 3.3427   -4 3.7143   -3 6.8100   -4                              "
4.31509  -2 7.9400   -3 5.4090   -4 7.8590   -4 3.0194   -3 1.7903   -2      "
5.8590   -4                                                                   "
3.1729   -4 1.6962   -3 6.9211   -5 4.4572   -5 1.5575   -2 1.7343   -3      "
5.5740   -2 9.7339   -3 1.2421   -3                                          "
    1     1     1     1                                                      #14
7.957747E-2                                                                    #15
    2    38                                                                    #16
0.23765E-07 0.21517E-03 0.64757E-04 0.54736E-03 0.35211E-02 0.87609E-02        #17
0.11237E-01 0.17710E-01 0.17130E-01 0.11876E-01 0.61696E-02 0.71458E-02        "
0.62605E-02 0.77929E-02 0.11490E-01 0.13724E-01 0.14378E-01 0.11571E-01        "
0.10887E-01 0.39651E-02 0.12242E-01 0.10692E-01 0.43725E-02 0.10106E-01        "
0.91849E-02 0.10760E-01 0.95585E-02 0.87266E-03 0.60139E-02 0.16505E-02        "
0.16275E-02 0.25313E-02 0.81854E-02 0.30115E-02 0.12102E-02 0.15625E-02        "
0.15258E-02
```

Fig.4.3 Example of input data for the BERMUDA-2DG

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
                                                                          #18
     1    40                                                              #19
 1.          1.          1.          1.          1.          1.            "
 1.          1.          1.          1.          1.          1.            "
 1.          1.          1.          1.          1.          1.            "
 1.          1.          1.          1.          1.          1.            "
 1.          1.          1.          1.          1.          1.            "
 1.          1.          1.          1.          1.          1.            "
 1.          1.          1.          1.                                    "
 @  MEASHB   MASS E. ABS. COEFF. (ERG*CM**2/G) HUBBEL                      #20
4.5961-73.7804-73.1919-72.8162-72.5409-72.3627-72.1855-72.0096-7           #21
1.8398-71.6755-71.5150-71.3577-71.2047-71.0552-79.1337-88.1140-8           "
7.4170-86.7314-86.1891-85.5201-85.1525-84.7763-84.3904-84.0239-8           "
3.6795-83.3207-82.9469-82.5889-82.4152-82.2963-82.0842-81.8165-8           "
1.6346-81.8111-82.6656-84.4734-87.1391-81.2261-73.0634-74.7910-7           "
1.1439-6
```

Fig.4.3 Example of input data for the BERMUDA-2DG (continued)

4.2.3 Output Data

The output data of BERMUDA-2DG are stored on the magnetic disk FT10 (Jxxxx.FLUX2DG.DATA; see Sec.4.2.1 (\$8)) and are also given on the printer.

The data on the output disk are as follows:

(1) In case of IPS≦0, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

(((PSI(JR,IZ,L),L＝1,LMAX),IZ＝1,NZMAX),JR＝1,NRMAX),
((TPSI(JR,IZ),IZ＝1,NZMAX),JR＝1,NRMAX),

where PSI(JR,IZ,L) : $\phi^{i}(r_{JR}, z_{IZ}, \vec{\Omega}_{L})$,

$$LMAX = \begin{cases} 40 \cdots \text{when calculation has been completed until the group IMAX,} \\ 48 \cdots \text{when calculation is to be restarted from the group } i_R+1, \end{cases}$$

NZMAX,NRMAX : see Sec.4.2.2 (#10) and

TPSI(JR,IZ) : $\Psi^{i}(r_{JR}, z_{IZ}) = \sum_{L=1}^{40} \Delta \vec{\Omega}_{L} \phi^{i}(r_{JR}, z_{IZ}, \vec{\Omega}_{L})$.

(2) In case of IPS≧1, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

(((PSI(JR,IZ,L),L＝1,LMAX),IZ＝1,NZMAX),JR＝1,NRMAX),
((PSI0(JR,IZ),IZ＝1,NZMAX),JR＝1,NRMAX),(PSI00(L),L＝1,40),
((TPSI(JR,IZ),IZ＝1,NZMAX),JR＝1,NRMAX),

where PSI(JR,IZ,L) : $\phi^{i}(r_{JR}, z_{IZ}, \vec{\Omega}_{L})$ (without component of uncollided flux),

LMAX,NZMAX,NRMAX : see above (1),

PSI0(JR,IZ) : $\Psi_{0}^{i}(r_{JR}, z_{IZ})$ (uncollided flux),

PSI00(L) : $S^{i}(0, z_{IZPS}, \vec{\Omega}_{L})$ (point source) and

$$\text{TPSI(JR, IZ)} : \Psi^{i}(r_{JR}, z_{IZ}) = \sum_{L=1}^{40} \Delta\vec{\Omega}_{L}\phi^{i}(r_{JR}, z_{IZ}, \vec{\Omega}_{L}) + \Psi_{0}^{i}(r_{JR}, z_{IZ}).$$

The data on the output print are as follows:

(a) list of input file Jxxxx.DATA2DG.DATA (see Sec.4.2.1 (\$5)) like Fig.4.3,

(b) list of the main input parameters with explanatory captions,

(The items (c)～(f) below are repeated for each energy group i (i＝1, …, IMAX).)

(c) CPU+VU time (sec) accumulated from the start of computation (EXEC LMGO) until the end of each main calculational item,

(d) when the convergence has been attained or ITMAX iterations have been finished for the 10-th grid,

- photon balance parameters; F, GAIN, ABBS, SELF, XLEK (see Sec.3.7 in Ref.1) integrated over the entire spatial region dealing with it as a single coarse mesh region,
- group no. i, iteration times IT, residual VERGF,

where $\text{VERGF} = \max_{JR, IZ, L} \left| \{\phi^{i(IT-1)}(r_{JR}, z_{IZ}, \vec{\Omega}_{L}) / \phi^{i(IT)}(r_{JR}, z_{IZ}, \vec{\Omega}_{L})\} - 1 \right| < \varepsilon$

(JR, IZ, L : except the cases where $\phi^{i(IT)}(r_{JR}, z_{IZ}, \vec{\Omega}_{L}) = 0$),

IT : iteration times (IT＝1, 2, …),

(As the energy grid model is used for all groups, these printed photon balance parameters and VERGF are meaningless, because the iteration is terminated by ITMAX (≦3) times. In addition, these parameters are obtained only from the data of the last (10-th) grid in the group i.)

(e) ・the upper energy boundary EUP(i) (eV),
・the lower energy boundary EUP(i+1) (eV),
・the energy width ΔE_i (eV),

(f) gamma rays scalar flux $\Psi^1(r_{JR}, z_{IZ})$ for JR＝1,…,10 and for IZ＝NZMIN,…,NZMAX,

where

$$NZMIN = \begin{cases} 1 \text{ for ISTEP} \neq 2, \\ \text{IFACE for ISTEP} = 2 \text{ (see Sec. 4. 2. 2 (\#2)) and} \end{cases}$$

(g) spatial distribution of reaction rate by input conversion factors (when NEWCF＝1) or dose rate (Sv/hr when NEWCF＝0)

$$\sum_{i=1}^{IMAX} CF(i)\Psi^1(r_{JR}, z_{IZ})$$

for JR＝1,…,10 and for IZ＝NZMIN,…,NZMAX, where CF is input new conversion factors (#21 in Sec. 4. 2. 2) or conversion factors installed in BERMUDA-2DG.

The STOP codes are as follows:

(1) 1001 : KMAX regions do not cover completely the whole (r, z) plane, or some regions overlap (error in J1(K), J2(K), I1(K) and I2(K) in input data #10),
(2) 2001 : IFACE in input data #02 is not on the bottom boundary of a partition in the z-direction and
(3) 2222 : The input fixed source for the group 1 is zero including the secondary gamma rays source.

4.3 BERMUDA-2DG-S16

4.3.1 JCL

The JCL for the BERMUDA-2DG-S16 execution on the FACOM/VP2600 computer in JAERI is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.14 W.06 C.00 I.10 E.12 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),CLASS=8,NOTIFY=Jxxxx (*1)
      OPTP PASSWORD=xxxxxxxx
//    EXEC LMGO,LM=J9091.BERMUDA,PNM=BM2DGS16,A='HIO=(01,09)' (*2)
//FT01F001 DD DISP=SHR,DSN=Jxxxx.FX701S16.DATA (*3)
//FT02F001 DD DISP=SHR,DSN=Jxxxx.BNDFGS16.DATA (*4)
//FT03F001 DD UNIT=WK10,SPACE=(TRK,(100,50)),DISP=(NEW,DELETE,DELETE),
//     DSN=&&WORK,DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
//FT04F001 DD DISP=SHR,DSN=J449B.BERM41G.DATA,LABEL=(,,,IN)
//SYSIN     DD DISP=SHR,DSN=Jxxxx.DT2DGS16.DATA (*5)
//FT08F001 DD DISP=SHR,DSN=Jxxxx.FX2DNS16.DATA (*6)
//FT09F001 DD DISP=SHR,DSN=Jxxxx.FX709S16.DATA (*7)
//FT10F001 DD DISP=SHR,DSN=Jxxxx.FX2DGS16.DATA (*8)
//FT11F001 DD DISP=SHR,DSN=Jxxxx.SB2DGS16.DATA (*9)
++
//
```

(*1) "CLASS=8" is a night job which needs an approval of the Computing and Information Systems Center of JAERI for submission. Besides this, there is the class 6 which also needs an approval but is not a night job. For this class 6, permitted CPU time (T.xx), print lines (W.xx) and I/O times (EXCP I.xx) have different values from those of the class 8.

(*2) There has already been a load module J9091.BERMUDA.LOAD(BM2DGS16) prepared for a public use in JAERI.

If necessary, a new load module is able to be created on a disk from the source module J9091.BERMUDA.FORT77(BM2DGS16). The JCL for creating a new load module is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
       T.02 W.03 C.02 I.02 E.00 SRP
       OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),NOTIFY=Jxxxx,PASSWORD=xxxxxxxx
//    EXEC FORT77VE,SO=J9091.BERMUDA,
//     A='ELM(BM2DGS16),SOURCE,NOVMSG,NOVSOURCE',LCT=62
//    EXEC LKEDCT77,LM=Jxxxx.BM2DGS16,UNIT=xxxxx,MODS='10,10,1',A=MAP
++
//
```

These steps of compilation and linkage are executed rather rapidly on the FACOM/M780 scalar computer. The new load module is applied by replacing the above "LM=J9091.BERMUDA,PNM=BM2DGS16" (\$2) with "LM=Jxxxx.BM2DGS16".

(\$3) The HIO (high-speed input/output) work file for the angular and scalar fluxes Jxxxx.FX701S16.DATA has to be allocated beforehand as:

```
//FT01F001 DD UNIT=TSSWK,SPACE=(CYL,280,,CONTIG),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FX701S16.DATA,
//     DCB=(RECFM=F,LRECL=23000,BLKSIZE=23000,DSORG=PS)
```

This file contains the spatial distributions of the angular and scalar photon fluxes for all of the calculated energy groups as a HIO work file for calculating the slowing down source from the upper energy groups.

So, this file can be deleted after the job has been successfully terminated in TMAX sec (see Sec.4.3.2) because the same data are stored in the FT10 (Jxxxx.FX2DGS16.DATA(\$8)) for restarting the job. The main purpose of the FT01(\$3) and FT09(\$7) is to utilize the HIO option for saving the I/O times (EXCP). In fact, the TSSWK is automatically deleted at 8:00 a.m. (the TSSWK2 at 5:00 p.m.) in JAERI. The HIO option needs to allocate the file

'contiguously' on the disk (CONTIG), and the FT01 and FT09 need to be allocated every time (or every day) before submitting the restarting job.

At the present, the specifications of the disk in JAERI are as follows:

1 VOL = 1,326 CYL × 2 (= 19,890 TRK × 2),

1 CYL = 15 TRK and

1 TRK = 47,476 bytes.

However, BLKSIZE cannot exceeds 32,767 bytes.

($4) The boundary flux file Jxxxx.BNDFGS16.DATA has to be allocated beforehand as:

```
//FT02F001 DD UNIT=xxxxx,SPACE=(TRK,(20,05)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.BNDFGS16.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the boundary flux in case of the bootstrap option (see Sec.3.6.2 in Ref.1). In the first step, the boundary flux is written in this file; and in the second step, the boundary flux is supplied from the file. When the bootstrap option is not used (ISTEP=0 in Sec.4.3.2), the one line of the JCL($4) is not necessary as well as allocation of the file.

($5) The input data file Jxxxx.DT2DGS16.DATA has to be allocated beforehand as:

```
//FT05F001 DD UNIT=xxxxx,SPACE=(TRK,(01,01)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.DT2DGS16.DATA,
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120,DSORG=PS)
```

The content of this file is described in Sec.4.3.2. Otherwise, the one line of the JCL($5) is substituted with

```
//SYSIN    DD *
     [input data described in Sec.4.3.2]
/*
```

without allocating the Jxxxx.DT2DGS16.DATA.

($6) The neutron flux file Jxxxx.FX2DNS16.DATA is an output file of BERMUDA-2DN-S16. If the problem does not need the secondary gamma rays source, the one line of the JCL($6) is substituted with the next one.

```
//FT08F001 DD DUMMY
```

($7) The HIO work file for the uncollided flux Jxxxx.FX709S16.DATA has to be allocated beforehand as:

```
//FT09F001 DD UNIT=TSSWK,SPACE=(CYL,03,,CONTIG),
//    DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FX709S16.DATA,
//    DCB=(RECFM=F,LRECL=23000,BLKSIZE=23000,DSORG=PS)
```

This file contains the spatial distribution of the uncollided gamma rays flux for all of the calculated energy groups as a HIO work file for calculating the first collision source from the self and the upper groups in Eq.(3.10).

This file can also be deleted same as the FT01 after the job has been successfully terminated in TMAX sec, because the same data are stored in the FT10 for restarting the job.

If IPS＝0, the one line of the JCL($7) is not necessary as well as allocation of the file.

($8) The gamma rays flux file Jxxxx.FX2DGS16.DATA has to be allocated beforehand as:

```
//FT10F001 DD  UNIT=xxxxx,SPACE=(TRK,(3800,100)),
//   DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FX2DGS16.DATA,
//   DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the spatial distributions of angular and scalar flux etc. of gamma rays for all of the calculated energy groups. It is used for restarting the job for energy group continuation and also can be used for editing the output results.

Note that the contents of the Jxxxx.FX2DGS16.DATA for the bootstrap step 1 vanish when the same file is used in the step 2. Usually comparison of the output data with the measured data concerns the region of the step 2. However, if it is necessary to save the data obtained in the step 1, dual files have to be allocated like Jxxxx.F2DGS161.DATA and Jxxxx.F2DGS162.DATA for each step.

($9) The grid source file Jxxxx.SB2DGS16.DATA has to be allocated beforehand as:

```
//FT11F001 DD UNIT=xxxxx,SPACE=(TRK,(950,50)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.SB2DGS16.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file is necessary for restarting the job as well as the FT10, and can be deleted after the calculation up to the IMAX-th group has been completed (in case of ISTEP≠0, up to the IMAX-th group in the step 2).
The contents of the FT11 are:

(1) the group no. i_R (Up to the i_R group the calculation has been completed.) and
(2) the grid source into the ten grids within the group i_R+1 from the groups 1 ～ i_R-1 and from the ten grids within the group i_R.

4.3.2 Input Data

#01 (F6.0) 1 line

・TMAX : CPU time (sec) to terminate the job and to prepare the disk files for restarting the next job (If CLASS＝8, then TMAX＝10000.)

#02 (4I3) 1 line

・IRSTRT : group no. to be restarted (initially ≡1)

・ISTEP : step no. for bootstrap option

$$ISTEP=\begin{cases}0 \cdots \text{no bootstrap option}\\ 1 \cdots \text{the first step}\\ 2 \cdots \text{the second step}\end{cases}$$

・IFACE : interface z-mesh point no. for bootstrap option (0 when ISTEP＝0) IFACE must be on the bottom boundary mesh point of a partition in the z-direction. (The numbering method for mesh points is described in #10.)
When ISTEP＝2, IFACE has a different value from that in ISTEP＝1.

・ITMAX : maximum number of iteration times for each energy grid (ITMAX＝1, 2 or 3)
(ITMAX is defined as 1, if 0 or blank is input.)

#03 (18A4) 1 line

・Problem title : any characters, numbers or blanks describing the problem on columns 1～72

#04 (9I4,2E12.5) 1 line

・IMAX : total number of energy groups for this problem (≦41)

・MMAX : number of mixtures (≦20)

・KMAX : number of spatial regions (MMAX≦KMAX)
Definition of a 'region' is that it is a rectangular part on the (r,z) plane, where mixture is assigned to be homogeneous.
The (r,z) plane must be completely covered with the KMAX regions.
Actually a 'region' is a ring-shaped volume made by rotating the rectangular around the axis of the cylinder (z＝0).

・I1L1B : group no. "on the group constants library" where the group 1 of this problem is to be defined

(for example, IMAX+I1LIB≦42 for J449B.BERM41G.DATA)

In BERMUDA, the I1LIB-th group on the library is called as "group 1".

・NILIB : initial group no. of the FT08 neutron flux file "on the neutron group constants library" (NILIB≡0 if FT08 is dummy.)

・NFLIB : final group no. of the FT08 neutron flux file "on the neutron group constants library" (NFLIB≡0 if FT08 is dummy.)
1≦NILIB≦NFLIB≦NMAXL and NFLIB-NILIB+1＝IMAXN (Sec.3.1)

・IPS : kind of the fixed source

$$IPS = \begin{cases} -1 \cdots \text{secondary gamma rays source only} \\ 0 \cdots \text{spatially distributed source} \\ IZPS \cdots \text{point source on the z-axis of the cylinder} \\ \qquad (IZPS \geqq 1) \end{cases}$$

The IZPS is the z-mesh point no. for the point source. When IZPS＝1, z(IZPS)＝0 (origin). The numbering method for the mesh points is described in #10. The point source cannot be placed on an interface between partitions in the z-direction.

・NRR : number of partitions in the r-direction (NRR≦20)
In each partition, mesh sizes (Δr) are assigned to be equal to each other.

・NRZ : number of partitions in the z-direction (NRZ≦20)
In each partition, mesh sizes (Δz) are assigned to be equal to each other.

・NEWCF : input of new conversion factors

$$NEWCF = \begin{cases} 0 \cdots \text{conversion factors prepared in the code are used.} \\ 1 \cdots \text{new conversion factors or responses are input in} \\ \qquad \text{the items \#20, 21 below and used.} \end{cases}$$

・IPSN : type of the fixed source for calculation of the FT08 neutron flux file

$$IPSN = \begin{cases} 0 \cdots \text{spatially distributed neutron source} \\ 1 \cdots \text{point neutron source} \end{cases}$$

・ER : upper energy (eV) for the group 1 of the problem
EUP(I1LIB+1)＜ER≦EUP(I1LIB)

・EPS : convergence criterion (for angular flux) to be used to terminate

the grid iteration before ITMAX (usually 10^{-3})

#05 (20I3) 1 line

・(MM(MK), MK＝1, MMAX) : number of nuclides to be included in each mixture
(1≦MM(MK)≦10)
(For a vacuum, assign one dummy nuclide which is contained in another mixture. Input its code number in #12 and atomic number density (0.) in #13.)

#06 (10I6) [(NRR+9)/10] lines

The brackets [⋯] means the integer discarding the fractions.

・(INTERR(KR), KR＝1, NRR) : number of mesh intervals between the origin and the outer boundary of each partition in the r-direction
(Either even or odd numbers are valid.)
(1≦INTERR(1)＜INTERR(2)＜⋯＜INTERR(NRR)≦60-NRR)

#07 (10F6.3) [(NRR+9)/10] lines

・(DRR(KR), KR＝1, NRR) : mesh size Δr (cm) for each partition in the r-direction
(not the partition thickness)

#08 (10I6) [(NRZ+9)/10] lines

・(INTERZ(KZ), KZ＝1, NRZ) : number of mesh intervals between the origin and the top boundary of each partition in the z-direction
(Either even or odd numbers are valid.)
(1≦INTERZ(1)＜INTERZ(2)＜⋯＜INTERZ(NRZ)≦110-NRZ)

#09 (10F6.3) [(NRZ+9)/10] lines

・(DZZ(KZ), KZ＝1, NRZ) : mesh size Δz (cm) for each partition in the z-direction
(not the partition thickness)

#10 (5I6) KMAX lines

・(J1(K), J2(K), I1(K), I2(K), MR(K), K＝1, KMAX) : assignment of composition
J1(K) : left mesh point no. of the region K

J2(K) : right mesh point no. of the region K
I1(K) : bottom mesh point no. of the region K
I2(K) : top mesh point no. of the region K
MR(K) : mixture no. for the region K (≡MK defined in #5)
(1≦J1<J2≦NRMAX≦60 and 1≦I1<I2≦NZMAX≦110)

In BERMUDA, the numbering of the mesh points is as follows:
(1) "1" for the origin,
(2) doubly (twice) numbered as "INTERR(KR)+KR" and "INTERR(KR)+KR+1" for the interface between the KR-th and the (KR+1)-th partitions in the r-direction where KR=1,…,NRR-1 (for treating spatial discontinuity of the macroscopic cross sections and the source distribution at the interfaces) and
(3) "NRMAX=INTERR(NRR)+NRR" ≦60 for the outermost mesh point in the r-direction.
And it is same for the z-direction except "NZMAX=INTERZ(NRZ)+NRZ" ≦110.

#11 (2F6.3) 1 line
・BCTOP : top boundary condition for z=z(NZMAX)
・BCBOT : bottom boundary condition for z=0.

$$\text{boundary conditions} \equiv \begin{cases} -1. & \cdots \text{ symmetry condition} \\ 0. & \cdots \text{ vacuum boundary condition} \end{cases}$$

#12 (1016) MMAX lines
・(MCODE(M,MK),M=1,MM(MK)) : code no. of each nuclide in the mixture MK defined in the group constants library to be used (see Sec.2.1)
(The order of nuclides in a mixture is able to be arbitrary.)
Repeat this in the order of MK=1,…,MMAX renewing the line for each mixture.

#13 (6E12.5) [(MM(MK)+5)/6] lines for each mixture
・(AN(M,MK),M=1,MM(MK)) : effective number density ($10^{24}cm^{-3}$) of each nuclide in the mixture MK
(The order of nuclides in a mixture must be same as in #12.)
Repeat this in the order of MK=1,…,MMAX renewing the line for each

mixture.

When IPS＝－1 in #04, data of #14～#19 below are not necessary to be input.

#14 (4I6) 1 line

- IZ1 : the first mesh point no. to give axial distribution of non-zero independent source in #15
- IZ2 : the last mesh point no. to give axial distribution of non-zero independent source in #15
- JR1 : the first mesh point no. to give radial distribution of non-zero independent source in #15
- JR2 : the last mesh point no. to give radial distribution of non-zero independent source in #15

  These mesh points must be given in the definition of (1)～(3) in #10 ($1 \leqq IZ1 \leqq IZ2 \leqq NZMAX$ and $1 \leqq JR1 \leqq JR2 \leqq NRMAX$). When IPS＝0 in #04, S1 in #15 is a volume source ($IZ1 < IZ2$ and $JR1 < JR2$). When $IPS \geqq 1$, S1 is a point source ($IZ1 = IZ2 = IPS$ and $JR1 = JR2 = 1$).

#15 (6E12.5) {[(JR2-JR1)/6]+1} lines

- (S1(JR,IZ),JR＝JR1,JR2) : spatial distribution of independent source

  Independent source is given in the form of a function with separation of variables as $S1(JR,IZ) \times S2(I) \times S3(L)$.

  (Each of the S1, S2 and S3 should be normalized to its correct magnitude, respectively. However, it is also valid that the product of the S1, S2 and S3 has the correct normalized value for each energy group(*).)

Repeat this in the order of IZ＝IZ1,…,IZ2.

#16 (2I6) 1 line

- I1 : the first energy group no. to give energy spectre of non-zero independent source in #17 (see Sec. 2. 2, but note that the group no. is defined so that the I1L1B-th group in Sec. 2. 2 is group 1.)
- I2 : the last energy group no. to give energy spectre of non-zero independent source in #17

  If the source is of mono-energy (monochromatic), I1＝I2＝1.

  Otherwise, $1 \leqq I1 < I2 \leqq IMAX$.

#17 (6E12.5)　　{[(I2-I1)/6]+1} lines

・(S2(I), I＝I1, I2) : energy spectre of independent source

(As BERMUDA has been programmed not in a continuous energy model but in a usual multigroup model, only the S2 (except the S1 and S3) must be given as integrated value for group i over ΔE_i.)

The S2(I) is generally normalized to be 1 integrated over energy, that is,

$$\sum_{I=I1}^{I2} S2(I) = 1.$$

(However, note the proviso(*) under #15.)

#18 (2I6)　　1 line

・L1 : the first ordinate no. to give angular distribution of non-zero independent source in #19 (see Fig.3.4 in Ref.1)

・L2 : the last ordinate no. to give angular distribution of non-zero independent source in #19

If the source is mono-directional, L1＝L2.

Otherwise, $1 \leqq L1 < L2 \leqq 144$. (S3(L) for L＝145,…,160 are assumed to have equal values to the adjacent (just right) ordinates, respectively.)

#19 (6E12.5)　　{[(L2-L1)/6]+1} lines

・(S3(L), L＝L1, L2) : angular distribution of independent source

The S3(L) is generally normalized to be 1 integrated over the unit sphere, that is,

$$\sum_{L=L1}^{L2} \Delta \vec{\Omega}_L S3(L) = 1.$$

(However, note the proviso(*) under #15.)

When NEWCF＝0 in #04, data of #20 and #21 below are not necessary to be input.

#20 (18A4)　　1 line

・Response name : any characters, numbers or blanks describing the conver-

sion factors given in #21 on columns 1～72

#21 (8F8.4)　　{[(NGMAX+7)/8]+1} lines

・(CF(I), I＝1, NGMAX) : conversion factors for 'all library groups'

An example of input data for the BERMUDA-2DG-S16 code is shown in Fig. 4. 4.

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
7000.                                                                          #01
 1  0  0  1                                                                   #02
SUS316 ASSEMBLY NUCLEAR HEATING 19/09/90 WED.                                  #03
 41   4  13   1   5 125   1   8   6   1   1 1.4      +7 5.0      -3            #04
 2 10  7  9                                                                    #05
    6     7     8    10    11    36    37    42                               #06
3.75  0.8   2.5   4.6   0.8  8.488 2.0   12.0                                  #07
   16    17    27    28    48    68                                           #08
15.5  2.0   7.8   1.6   3.0   3.0                                             #09
    1    42     1    17     1    REG 1 AIR FRONT PART                         #10
   43    44     1    17     2    REG 2 MORTAR                                  "
   45    50     1    19     3    REG 3 ROOM WALL                               "
    1    14    18    30     1    REG 1-2 AIR FRONT PART                        "
   15    16    18    32     4    REG 4 FE TEST PORT FLAME                      "
   17    44    18    19     2    REG 2-2 MORTAR                                "
   17    50    20    32     3    REG 3-2 ROOM WALL                             "
    1     7    31    32     1    REG 1-3 AIR FRONT PART                        "
    8    14    31    32     4    REG 4-2 FE TEST PORT FLAME                    "
    1     9    33    53     4    REG 4-3 FE TEST PORT SUS316                   "
   10    50    33    53     3    REG 3-3 ROOM WALL                             "
    1    11    54    74     4    REG 4-4 FE TEST PORT SUS316                   "
   12    50    54    74     3    REG 3-4 ROOM WALL                             "
0.   -1.                                                                       #11
  707   807                                                                    #12
  117   807   807  1307  1307  1307  1407  1407  1407  2607                    "
  807   117  1307  1307  1307  1407  2607                                      "
  607  1407  1407  1407  2407  2507  2607  2807  4207                          "
4.2000   -5 1.1300   -5                                                       #13
9.4246   -3 7.4297   -4 3.7680   -2 5.0802   -4 4.6874   -4 1.9408   -3       "
1.1347   -2 3.3427   -4 3.7143   -3 6.8100   -4                               "
4.31509  -2 7.9400   -3 5.4090   -4 7.8590   -4 3.0194   -3 1.7903   -2       "
5.8590   -4                                                                    "
3.1729   -4 1.6962   -3 6.9211   -5 4.4572   -5 1.5575   -2 1.7343   -3       "
5.5740   -2 9.7339   -3 1.2421   -3                                           "
    1     1     1     1                                                       #14
7.957747E-2                                                                   #15
    2    38                                                                   #16
0.23765E-07 0.21517E-03 0.64757E-04 0.54736E-03 0.35211E-02 0.87609E-02       #17
0.11237E-01 0.17710E-01 0.17130E-01 0.11876E-01 0.61696E-02 0.71458E-02        "
0.62605E-02 0.77929E-02 0.11490E-01 0.13724E-01 0.14378E-01 0.11571E-01        "
0.10887E-01 0.39651E-02 0.12242E-01 0.10692E-01 0.43725E-02 0.10106E-01        "
0.91849E-02 0.10760E-01 0.95585E-02 0.87266E-03 0.60139E-02 0.16505E-02        "
0.16275E-02 0.25313E-02 0.81854E-02 0.30115E-02 0.12102E-02 0.15625E-02        "
0.15258E-02                                                                    "
```

Fig.4.4 Example of input data for the BERMUDA-2DG-S16

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8

        1    144                                                            #18
1.           1.           1.           1.           1.           1.         #19
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
1.           1.           1.           1.           1.           1.          "
@  MEASHB   MASS E. ABS. COEFF. (ERG*CM**2/G) HUBBEL                        #20
4.5961-73.7804-73.1919-72.8162-72.5409-72.3627-72.1855-72.0096-7            #21
1.8398-71.6755-71.5150-71.3577-71.2047-71.0552-79.1337-88.1140-8             "
7.4170-86.7314-86.1891-85.5201-85.1525-84.7763-84.3904-84.0239-8             "
3.6795-83.3207-82.9469-82.5889-82.4152-82.2963-82.0842-81.8165-8             "
1.6346-81.8111-82.6656-84.4734-87.1391-81.2261-73.0634-74.7910-7             "
1.1439-6
```

Fig.4.4 Example of input data for the BERMUDA-2DG-S16 (continued)

4.3.3 Output Data

The output data of BERMUDA-2DG-S16 are stored on the magnetic disk FT10 (Jxxxx.FX2DGS16.DATA; see Sec.4.3.1 ($8)) and are also given on the printer.

The data on the output disk are as follows:

(1) In case of IPS≦0, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

(((PSI(JR,IZ,L),L＝1,LMAX),IZ＝1,NZMAX),JR＝1,NRMAX),
((TPSI(JR,IZ),IZ＝1,NZMAX),JR＝1,NRMAX),

where PSI(JR,IZ,L) : $\phi^i(r_{JR}, z_{IZ}, \vec{\Omega}_L)$,

$$LMAX = \begin{cases} 144\cdots \text{when calculation has been completed until the group IMAX,} \\ 160\cdots \text{when calculation is to be restarted from the group } i_R+1, \end{cases}$$

NZMAX,NRMAX : see Sec.4.3.2 (#10) and

TPSI(JR,IZ) : $\Psi^i(r_{JR}, z_{IZ}) = \sum_{L=1}^{144} \Delta\vec{\Omega}_L \phi^i(r_{JR}, z_{IZ}, \vec{\Omega}_L)$.

(2) In case of IPS≧1, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

(((PSI(JR,IZ,L),L＝1,LMAX),IZ＝1,NZMAX),JR＝1,NRMAX),
((PSI0(JR,IZ),IZ＝1,NZMAX),JR＝1,NRMAX),(PSI00(L),L＝1,40),
((TPSI(JR,IZ),IZ＝1,NZMAX),JR＝1,NRMAX),

where PSI(JR,IZ,L) : $\phi^i(r_{JR}, z_{IZ}, \vec{\Omega}_L)$ (without component of uncollided flux),

LMAX,NZMAX,NRMAX : see above (1),

PSI0(JR,IZ) : $\Psi_0^i(r_{JR}, z_{IZ})$ (uncollided flux),

PSI00(L) : $S^i(0, z_{IZPS}, \vec{\Omega}_L)$ (point source) and

$$\mathrm{TPSI(JR,IZ)}\ :\ \Psi^{i}(r_{JR},z_{IZ})=\sum_{L=1}^{144}\Delta\vec{\Omega}_{L}\phi^{i}(r_{JR},z_{IZ},\vec{\Omega}_{L})$$
$$+\Psi_{0}^{i}(r_{JR},z_{IZ}).$$

The data on the output print are as follows:

(a) list of input file Jxxxx.DT2DGS16.DATA (see Sec.4.3.1 ($5)) like Fig.4.4,
(b) list of the main input parameters with explanatory captions,

(The items (c)～(f) below are repeated for each energy group i (i＝1, …, IMAX).)

(c) CPU+VU time (sec) accumulated from the start of computation (EXEC LMGO) until the end of each main calculational item,
(d) when the convergence has been attained or ITMAX iterations have been finished for the 10-th grid,
- photon balance parameters; F, GAIN, ABBS, SELF, XLEK (see Sec.3.7 in Ref.1) integrated over the entire spatial region dealing with it as a single coarse mesh region,
- group no. i, iteration times IT, residual VERGF,

where $\mathrm{VERGF}=\max_{JR,IZ,L}\left|\left\{\phi^{i(IT-1)}(r_{JR},z_{IZ},\vec{\Omega}_{L})/\phi^{i(IT)}(r_{JR},z_{IZ},\vec{\Omega}_{L})\right\}-1\right|<\varepsilon$

(JR,IZ,L : except the cases where $\phi^{i(IT)}(r_{JR},z_{IZ},\vec{\Omega}_{L})=0$),
IT : iteration times (IT＝1, 2, …),

(As the energy grid model is used for all groups, these printed photon balance parameters and VERGF are meaningless, because the iteration is terminated by ITMAX (≦3) times. In addition, these parameters are obtained only from the data of the last (10-th) grid in the group i.)

(e) ・the upper energy boundary EUP(i) (eV),
・the lower energy boundary EUP(i+1) (eV),
・the energy width ΔE_i (eV),

(f) gamma rays scalar flux $\Psi^1(r_{JR}, z_{IZ})$ for JR＝1,…,10 and for IZ＝NZMIN,…,NZMAX,

where

$$NZMIN = \begin{cases} 1 \text{ for ISTEP} \neq 2, \\ \text{IFACE for ISTEP} = 2 \text{ (see Sec. 4.3.2 (\#2)) and} \end{cases}$$

(g) spatial distribution of reaction rate by input conversion factors (when NEWCF＝1) or dose rate (Sv/hr when NEWCF＝0)

$$\sum_{i=1}^{IMAX} CF(i)\Psi^1(r_{JR}, z_{IZ})$$

for JR＝1,…,10 and for IZ＝NZMIN,…,NZMAX, where CF is input new conversion factors (#21 in Sec. 4.3.2) or conversion factors installed in BERMUDA-2DG-S16.

The STOP codes are as follows:

(1) 1001 : KMAX regions do not cover completely the whole (r,z) plane, or some regions overlap (error in J1(K), J2(K), I1(K) and I2(K) in input data #10),
(2) 2001 : IFACE in input data #02 is not on the bottom boundary of a partition in the z-direction and
(3) 2222 : The input fixed source for the group 1 is zero including the secondary gamma rays source.

4.4 BERMUDA-3DG

4.4.1 JCL

The JCL for the BERMUDA-3DG execution on the FACOM/VP2600 computer in JAERI is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
       T.15 W.09 C.00 I.15 E.44 SRP
       T=(1440,00)
       OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),CLASS=9,NOTIFY=Jxxxx (*1)
       OPTP PASSWORD=xxxxxxxx
//    EXEC LMGO,LM=J9091.BERMUDA,PNM=BERMD3DG,A='HIO=(01)' (*2)
//FT01F001 DD DISP=SHR,DSN=Jxxxx.FLX701.DATA (*3)
//FT02F001 DD DISP=SHR,DSN=Jxxxx.BOUNDFXG.DATA (*4)
//FT03F001 DD UNIT=WK10,SPACE=(TRK,(100,50)),DISP=(NEW,DELETE,DELETE),
//     DSN=&&WORK,DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
//FT04F001 DD DISP=SHR,DSN=J449B.BERM41G.DATA,LABEL=(,,,IN)
//SYSIN     DD DISP=SHR,DSN=Jxxxx.DATA3DG.DATA (*5)
//FT08F001 DD DISP=SHR,DSN=Jxxxx.FLUX3DN.DATA (*6)
//FT09F001 DD DISP=SHR,DSN=Jxxxx.FLUX3DG.DATA (*7)
//FT10F001 DD DISP=SHR,DSN=Jxxxx.SDB3DG.DATA (*8)
++
//
```

(*1) "CLASS=9" is a specially reserved job for occupying the almost all of the '500MB extended memory' (that is, 440MB (E.44)) and the FACOM/VP2600 computer through one day or more.

So, this is a closed job for 'a weekend' once a month or once per two months, and the Jxxxx may be a personnel no. of some staff in the Computing and Information Systems Center of JAERI.

'T.15' is dummy and 'T=(1440,00)' means that CPU+VU time may be unlimited until the next Monday morning.

(\$2) There has already been a load module J9091.BERMUDA.LOAD(BERMD3DG) prepared for a public use in JAERI.

If necessary, a new load module is able to be created on a disk from the source module J9091.BERMUDA.FORT77(BERMD3DG). The JCL for creating a new load module is as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER xxxxxxxx,xx.xxxxxxxx,xxxx.xx
      T.02 W.03 C.02 I.02 E.00 SRP
      OPTP MSGCLASS=X,MSGLEVEL=(1,1,2),NOTIFY=Jxxxx,PASSWORD=xxxxxxxx
//    EXEC FORT77VE,SO=J9091.BERMUDA,
//     A='ELM(BERMD3DG),SOURCE,NOVMSG,NOVSOURCE',LCT=62
//    EXEC LKEDCT77,LM=Jxxxx.BERMD3DG,UNIT=xxxxx,MODS='11,11,1',A=MAP
++
//
```

These steps of compilation and linkage are executed rather rapidly on the FACOM/M780 scalar computer. The new load module is applied by replacing the above "LM=J9091.BERMUDA,PNM=BERMD3DG" (\$2) with "LM=Jxxxx.BERMD3DG".

(\$3) The HIO (high-speed input/output) work file for the angular and scalar fluxes Jxxxx.FLX701.DATA has to be allocated beforehand as:

```
//FT01F001 DD UNIT=TSSWK,SPACE=(CYL,1100,,CONTIG),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLX701.DATA,
//     DCB=(RECFM=F,LRECL=23000,BLKSIZE=23000,DSORG=PS)
```

This file contains the spatial distributions of the angular and scalar photon fluxes for all of the calculated energy groups as a HIO work file for calculating the slowing down source from these energy groups.

So, this file can be deleted after the job has been successfully terminated, because the same data are stored in the FT09 (Jxxxx.FLUX3DG.DATA(\$7)) for output data edition. The main purpose of the FT01(\$3) is to utilize the HIO option for saving the I/O times (EXCP). In fact, the TSSWK is automati-

cally deleted at 8:00 a.m. on the next Monday. The HIO option needs to allocate the file 'contiguously' on the disk (CONTIG), and the FT0i needs to be allocated every time before executing the special large job.

At the present, the specifications of the disk in JAERI are as follows:

1 VOL = 1,326 CYL × 2 (= 19,890 TRK × 2),

1 CYL = 15 TRK and

1 TRK = 47,476 bytes.

However, BLKSIZE cannot exceeds 32,767 bytes.

($4) The boundary flux file Jxxxx.BOUNDFXG.DATA has to be allocated beforehand as:

```
//FT02F001 DD UNIT=xxxxx,SPACE=(TRK,(130,10)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.BOUNDFXG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the boundary flux in case of the bootstrap option (see Sec.3.6.2 in Ref.1). In the first step, the boundary flux is written in this file; and in the second step, the boundary flux is supplied from the file. When the bootstrap option is not used (ISTEP＝0 in Sec.4.4.2), the one line of the JCL($4) is not necessary as well as allocation of the file.

($5) The input data file Jxxxx.DATA3DG.DATA has to be allocated beforehand as:

```
//FT05F001 DD UNIT=xxxxx,SPACE=(TRK,(01,01)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.DATA3DG.DATA,
//     DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120,DSORG=PS)
```

The content of this file is described in Sec.4.4.2. Otherwise, the one line of the JCL($5) is substituted with

```
//SYSIN    DD *
     [input data described in Sec.4.4.2]
/*
```

without allocating the Jxxxx.DATA3DG.DATA.

($6) The neutron flux file Jxxxx.FLUX3DN.DATA is an output file of BERMUDA-3DN. If the problem does not need the secondary gamma rays source, the one line of the JCL($6) is substituted with the next one.

```
//FT08F001 DD DUMMY
```

($7) The gamma rays flux file Jxxxx.FLUX3DG.DATA has to be allocated as:

```
//FT09F001 DD UNIT=xxxxx,SPACE=(TRK,(15300,100)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.FLUX3DG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file contains the spatial distributions of angular and scalar flux of gamma rays for all of the calculated energy groups. It can be used for restarting the job for energy group continuation and also for editing the output results.

Note that the contents of the Jxxxx.FLUX3DG.DATA for the bootstrap step 1 vanish when the same file is used in the step 2. Usually comparison of the output data with the measured data concerns the region of the step 2. However, if it is necessary to save the data obtained in the step 1, dual files have to be allocated as Jxxxx.FLUX3DG1.DATA and Jxxxx.FLUX3DG2.DATA for each step.

($8) The grid source file Jxxxx.SDB3DG.DATA has to be allocated beforehand as:

```
//FT10F001 DD UNIT=xxxxx,SPACE=(TRK,(3700,100)),
//     DISP=(NEW,CATLG,CATLG),DSN=Jxxxx.SDB3DG.DATA,
//     DCB=(RECFM=VBS,LRECL=23472,BLKSIZE=23476,DSORG=PS)
```

This file can be used for restarting the job as well as FT09, and can be deleted after the calculation up to the IMAX-th group has been completed (in case of ISTEP≠0, up to the IMAX-th group in the step 2).

The contents of the FT10 are:

(1) the group no. i_R (Up to the i_R group the calculation has been completed.) and

(2) the grid source into the ten grids within the group i_R+1 from the groups 1 ～ i_R-1 and from the ten grids within the group i_R.

4.4.2 Input Data

#01 (F6.0) 1 line

・TMAX : CPU time (sec) to terminate the job and to prepare the disk files for restarting the next job (If CLASS＝9, then TMAX＝1.0E+6)

#02 (4I3) 1 line

・IRSTRT : group no. to be restarted (initially ≡1)

・ISTEP : step no. for bootstrap option

$$ISTEP=\begin{cases}0 \cdots \text{no bootstrap option}\\ 1 \cdots \text{the first step}\\ 2 \cdots \text{the second step}\end{cases}$$

・IFACE : interface z-mesh point no. for bootstrap option (0 when ISTEP＝0)
IFACE must be on the bottom boundary mesh point of a partition in the z-direction. (The numbering method for mesh points is described in #12.)
When ISTEP＝2, IFACE has a different value from that in ISTEP＝1.

・ITMAX : maximum number of iteration times for each energy grid
(ITMAX＝1, 2 or 3)
(ITMAX is defined as 1, if 0 or blank is input.)

#03 (18A4) 1 line

・Problem title : any characters, numbers or blanks describing the problem on columns 1～72

#04 (1I14, 2E12.5) 1 line

・IMAX : total number of energy groups for this problem (≦41)

・MMAX : number of mixtures (≦20)

・KMAX : number of spatial regions (MMAX≦KMAX)
Definition of a 'region' is that it is a rectangular parallelpiped part in the (x, y, z) whole volume, where mixture is assigned to be homogeneous.
The (x, y, z) whole volume must be completely filled up with the KMAX regions.

・I1LIB : group no. "on the group constants library" where the group 1 of this problem is to be defined

(for example, IMAX+I1LIB≦42 for J449B.BERM41G.DATA)

In BERMUDA, the I1LIB-th group on the library is called as "group 1".

・NILIB : initial group no. of the FT08 neutron flux file "on the neutron group constants library" (NILIB＝0 if FT08 is dummy.)

・NFLIB : final group no. of the FT08 neutron flux file "on the neutron group constants library" (NFLIB＝0 if FT08 is dummy.)
1≦NILIB≦NFLIB≦NMAXL and NFLIB-NILIB+1＝IMAXN (Sec.3.1)

・IPS : type of the fixed source

$$IPS=\begin{cases} -1 \cdots \text{secondary gamma rays source only} \\ 0 \cdots \text{spatially distributed source} \\ IYPS \cdots \text{point source on the y-axis of the rectangular parallelpiped } (IYPS \geqq 1) \end{cases}$$

The IYPS is the y-mesh point no. for the point source. When IYPS＝1, y(IYPS)＝0 (origin). The numbering method for the mesh points is described in #12. The point source cannot be placed on an interface between partitions in the y-direction.

・NRX : number of partitions in the x-direction (NRX≦20)
In each partition, mesh sizes (Δx) are assigned to be equal to each other.

・NRY : number of partitions in the y-direction (NRY≦20)
In each partition, mesh sizes (Δy) are assigned to be equal to each other.

・NRZ : number of partitions in the z-direction (NRZ≦20)
In each partition, mesh sizes (Δz) are assigned to be equal to each other.

・NEWCF : input of new conversion factors

$$NEWCF=\begin{cases} 0 \cdots \text{conversion factors prepared in the code are used.} \\ 1 \cdots \text{new conversion factors or responses are input in the items \#22,23 below and used.} \end{cases}$$

・ER : upper energy (eV) for the group 1 of the problem
EUP(I1LIB+1)＜ER≦EUP(I1LIB)

・EPS : convergence criterion (for angular flux) to be used to terminate the grid iteration before ITMAX (usually 10^{-3})

#05 (20I3) 1 line

・(MM(MK), MK＝1, MMAX) : number of nuclides to be included in each mixture
(1≦MM(MK)≦10)
(For a vacuum, assign one dummy nuclide which is contained in another mixture. Input its code number in #14 and atomic number density (0.) in #15.)

#06 (10I6) [(NRX+9)/10] lines

The brackets [⋯] means the integer discarding the fractions.

・(INTERX(KX), KX＝1, NRX) : number of mesh intervals between the origin and the front boundary of each partition in the x-direction
(Either even or odd numbers are valid.)
(1≦INTERX(1)＜INTERX(2)＜⋯＜INTERX(NRX)≦30-NRX)

The origin is placed at the back, left and bottom corner of the volume to be dealt with.

#07 (10F6.3) [(NRX+9)/10] lines

・(DXX(KX), KX＝1, NRX) : mesh size Δx (cm) for each partition in the x-direction
(not the partition thickness)

#08 (10I6) [(NRY+9)/10] lines

・(INTERY(KY), KY＝1, NRY) : number of mesh intervals between the origin and the right boundary of each partition in the y-direction
(Either even or odd numbers are valid.)
(1≦INTERY(1)＜INTERY(2)＜⋯＜INTERY(NRY)≦30-NRY)

#09 (10F6.3) [(NRY+9)/10] lines

・(DYY(KY), KY＝1, NRY) : mesh size Δy (cm) for each partition in the y-direction
(not the partition thickness)

#10 (10I6) [(NRZ+9)/10] lines

・(INTERZ(KZ), KZ=1, NRZ) : number of mesh intervals between the origin and the top boundary of each partition in the z-direction
(Either even or odd numbers are valid.)
(1≦INTERZ(1)<INTERZ(2)<…<INTERZ(NRZ)≦60-NRZ)

#11 (10F6.3) [(NRZ+9)/10] lines

・(DZZ(KZ), KZ=1, NRZ) : mesh size Δz (cm) for each partition in the z-direction
(not the partition thickness)

#12 (7I6) KMAX lines

・(KX1(K), KX2(K), JY1(K), JY2(K), IZ1(K), IZ2(K), MR(K), K=1, KMAX) : assignment of composition
KX1(K) : back mesh point no. of the region K
KX2(K) : front mesh point no. of the region K
JY1(K) : left mesh point no. of the region K
JY2(K) : right mesh point no. of the region K
IZ1(K) : bottom mesh point no. of the region K
IZ2(K) : top mesh point no. of the region K
MR(K) : mixture no. for the region K (≡MK defined in #5)
(1≦KX1<KX2≦NXMAX≦30, 1≦JY1<JY2≦NYMAX≦30 and 1≦IZ1<IZ2≦NZMAX≦60)

In BERMUDA, the numbering of the mesh points is as follows:

(1) "1" for the origin,

(2) doubly (twice) numbered as "INTERX(KX)+KX" and "INTERX(KX)+KX+1" for the interface between the KX-th and the (KX+1)-th partitions in the x-direction where KX=1,…,NRX-1 (for treating spatial discontinuity of the macroscopic cross sections and the source distribution at the interfaces) and

(3) "NXMAX=INTERX(NRX)+NRX" ≦30 for the outermost mesh point in the x-direction.

And it is same for the y-direction, "NYMAX=INTERY(NRY)+NRY" ≦30 and also same for the z-direction except "NZMAX=INTERZ(NRZ)+NRZ" ≦60.

#13 (6F6.3) 1 line

・BCX1 : back boundary condition for x＝0.

・BCX2 : front boundary condition for x＝x(NXMAX)

・BCY1 : left boundary condition for y＝0.

・BCY2 : right boundary condition for y＝y(NYMAX)

・BCZ1 : bottom boundary condition for z＝0.

・BCZ2 : top boundary condition for z＝z(NZMAX)

$$\text{boundary conditions} \equiv \begin{cases} -1. & \cdots \text{ symmetry condition} \\ 0. & \cdots \text{ vacuum boundary condition} \end{cases}$$

#14 (10I6) MMAX lines

・(MCODE(M,MK),M＝1,MM(MK)) : code no. of each nuclide in the mixture MK defined in the group constants library to be used (see Sec.2.1) (The order of nuclides in a mixture is able to be arbitrary.)

Repeat this in the order of MK＝1,…,MMAX renewing the line for each mixture.

#15 (6E12.5) [(MM(MK)+5)/6] lines for each mixture

・(AN(M,MK),M＝1,MM(MK)) : effective number density ($10^{24}cm^{-3}$) of each nuclide in the mixture MK (The order of nuclides in a mixture must be same as in #14.)

Repeat this in the order of MK＝1,…,MMAX renewing the line for each mixture.

When IPS＝-1 in #04, data of #16～#21 below are not necessary to be input.

#16 (6I6) 1 line

・KXS1 : the first mesh point no. to give x-distribution of non-zero independent source in #17

・KXS2 : the last mesh point no. to give x-distribution of non-zero independent source in #17

・JYS1 : the first mesh point no. to give y-distribution of non-zero independent source in #17

・JYS2 : the last mesh point no. to give y-distribution of non-zero independent source in #17

・IZS1 : the first mesh point no. to give z-distribution of non-zero

independent source in #17

・IZS2 : the last mesh point no. to give z-distribution of non-zero independent source in #17
These mesh points must be given in the definition of (1)～(3) in #12 ($1 \leqq KXS1 \leqq KXS2 \leqq NXMAX$, $1 \leqq JYS1 \leqq JYS2 \leqq NYMAX$ and $1 \leqq IZS1 \leqq IZS2 \leqq NZMAX$).
When IPS＝0 in #04, S1 in #17 is a volume source ($KXS1 < KXS2$, $JYS1 < JYS2$ and $IZS1 < IZS2$). When $IPS \geqq 1$, S1 is a point source ($KXS1 = KXS2 = 1$, $JYS1 = JYS2 = IPS$ and $IZS1 = IZS2 = 1$).

#17 (6E12.5) {[(JYS2-JYS1)/6]+1} lines for each (KX, IZ) point

・(S1(KX, JY, IZ), JY＝JYS1, JYS2) : spatial distribution of independent source
Independent source is given in the form of a function with separation of variables as $S1(KX, JY, IZ) \times S2(I) \times S3(L)$.
(Each of the S1, S2 and S3 should be normalized to its correct magnitude, respectively. However, it is also valid that the product of the S1, S2 and S3 has the correct normalized value for each energy group(*).)

Repeat it in the order of KX＝KXS1, …, KXS2 renewing the line for each KX.

And repeat "the above set over JY and KX" in the order of IZ＝IZS1, …, IZS2.

#18 (2I6) 1 line

・I1 : the first energy group no. to give energy spectre of non-zero independent source in #19 (see Sec. 2.2, but note that the group no. is defined so that the I1LIB-th group in Sec. 2.2 is group 1.)

・I2 : the last energy group no. to give energy spectre of non-zero independent source in #19
If the source is of mono-energy (monochromatic), I1＝I2＝1.
Otherwise, $1 \leqq I1 < I2 \leqq IMAX$.

#19 (6E12.5) {[(I2-I1)/6]+1} lines

・(S2(I), I＝I1, I2) : energy spectre of independent source
(As BERMUDA has been programmed not in a continuous energy model but in a usual multigroup model, only the S2 (except the S1 and S3) must be given as integrated value for group i over ΔE_i.)

The S2(I) is generally normalized to be 1 integrated over energy, that is,

$$\sum_{I=I1}^{I2} S2(I) = 1.$$

(However, note the proviso(*) under #17.)

#20 (2I6) 1 line

- L1 : the first ordinate no. to give angular distribution of non-zero independent source in #21 (see Fig.3.6 in Ref.1)
- L2 : the last ordinate no. to give angular distribution of non-zero independent source in #21
  If the source is mono-directional, L1=L2.
  Otherwise, $1 \leqq L1 < L2 \leqq 80$.

#21 (6E12.5) {[(L2-L1)/6]+1} lines

- (S3(L), L=L1, L2) : angular distribution of independent source
  The S3(L) is generally normalized to be 1 integrated over the unit sphere, that is,

$$\sum_{L=L1}^{L2} \Delta \vec{\Omega}_L S3(L) = 1.$$

(However, note the proviso(*) under #17.)

When NEWCF=0 in #04, data of #22 and #23 below are not necessary to be input.

#22 (18A4) 1 line

- Response name : any characters, numbers or blanks describing the conversion factors given in #23 on columns 1～72

#23 (8f8.4) {[(NGMAX+7)/8]+1} lines

- (CF(I), I=1, NGMAX) : conversion factors for 'all library groups'

4.4.3 Output Data

The output data of the BERMUDA-3DG are stored on the magnetic disk FT09 (Jxxxx.FLUX3DG.DATA; see Sec.4.4.1 (\$7)) and are also given on the printer.

The data on the output disk are as follows:

(1) In case of IPS≦0, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

((((PSI(KX,JY,IZ,L),L＝1,80),IZ＝1,NZMAX),JY＝1,NYMAX),KX＝1,NXMAX),
(((TPSI(KX,JY,IZ),IZ＝1,NZMAX),JY＝1,NYMAX),KX＝1,NXMAX),

where PSI(KX,JY,IZ,L) : $\phi^{i}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_{L})$,
TPSI(KX,JY,IZ) : $\Psi^{i}(x_{KX}, y_{JY}, z_{IZ})$

$$= \sum_{L=1}^{80} \Delta\vec{\Omega}_{L}\phi^{i}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_{L}) \text{ and}$$

NXMAX,NYMAX,NZMAX : see Sec.4.4.2 (#12).

(2) In case of IPS≧1, the following FORTRAN record is repeated for each group i (i＝1,…,IMAX) in the binary form,

((((PSI(KX,JY,IZ,L),L＝1,80),IZ＝1,NZMAX),JY＝1,NYMAX),KX＝1,NXMAX),
(((TPSI(KX,JY,IZ),IZ＝1,NZMAX),JY＝1,NYMAX),KX＝1,NXMAX),

where PSI(1,1,NZMAX,L) : $\phi^{i}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_{L}) + \phi_{0}^{i}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_{L})$,
TPSI(KX,JY,IZ) : $\Psi^{i}(x_{KX}, y_{JY}, z_{IZ})$

$$= \sum_{L=1}^{80} \Delta\vec{\Omega}_{L}\{\phi^{i}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_{L}) + \phi_{0}^{i}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_{L})\} \text{ and}$$

NXMAX,NYMAX,NZMAX : see above (1).

The data on the output print are as follows:

(a) list of input file Jxxxx.DATA3DG.DATA (see Sec.4.4.1 (\$5)),

(b) list of the main input parameters with explanatory captions,

(The items (c)～(g) below are repeated for each energy group i (i＝1, …, IMAX).)

(c) CPU+VU time (sec) accumulated from the start of computation (EXEC LMGO) until the end of each main calculational item,

(d) when the convergence has been attained or ITMAX iterations have been finished for the 10-th grid,

- photon balance parameters; F, GAIN, ABBS, SELF, XLEK (see Sec.3.7 in Ref.1) integrated over the entire spatial region dealing with it as a single coarse mesh region,
- group no. i, iteration times IT, residual VERGF,

where $VERGF = \max_{KX, JY, IZ, L} \left| \left\{ \phi^{i(IT-1)}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_L) / \phi^{i(IT)}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_L) \right\} - 1 \right| < \varepsilon$

(KX, JY, IZ, L : except the cases where $\phi^{i(IT)}(x_{KX}, y_{JY}, z_{IZ}, \vec{\Omega}_L) = 0$),

IT : iteration times (IT＝1, 2, …),

(As the energy grid model is used for all groups, these printed photon balance parameters and VERGF are meaningless, because the iteration is terminated by ITMAX (≦3) times. In addition, these parameters are obtained only from the data of the last (10-th) grid in the group i.)

(e) - the upper energy boundary EUP(i) (eV),
- the lower energy boundary EUP(i+1) (eV),
- the energy width ΔE_i (eV),

(f) gamma rays scalar flux over the x＝0 plane, $\Psi^i(0, y_{JY}, z_{IZ})$ for JY＝1, …, NYMAX and for IZ＝NZMIN, …, NZMAX,

where

$$NZMIN = \begin{cases} 1 & \text{for ISTEP} \neq 2, \\ IFACE & \text{for ISTEP} = 2 \text{ (see Sec.4.4.2 (\#2)),} \end{cases}$$

(g) gamma rays scalar flux over the $z = z_{NZMAX}$ plane, $\Psi^i(x_{KX}, y_{JY}, z_{NZMAX})$ for KX＝1,…,NXMAX and for JY＝1,…,NYMAX.

(h) spatial distribution of reaction rate by input conversion factors (when NEWCF＝1) or dose rate (Sv/hr when NEWCF＝0) over the x＝0 plane

$$\sum_{i=1}^{IMAX} CF(i)\Psi^i(0, y_{JY}, z_{IZ})$$

for JY＝1,…,NYMAX and for IZ＝NZMIN,…,NZMAX, where CF is input new conversion factors (#23 in Sec.4.4.2) or conversion factors installed in BERMUDA-3DG, and

(i) spatial distribution of reaction rate by input conversion factors (when NEWCF＝1) or dose rate (Sv/hr when NEWCF＝0) over the $z = z_{NZMAX}$ plane

$$\sum_{i=1}^{IMAX} CF(i)\Psi^i(x_{KX}, y_{JY}, z_{NZMAX})$$

for KX＝1,…,NXMAX and for JY＝1,…,NYMAX.

The STOP codes are as follows:

(1) 1001 : KMAX regions do not cover completely the whole (x,y,z) volume, or some regions overlap (error in KX1(K),KX2(K), JY1(K), JY2(K), IZ1(K) and IZ2(K) in input data #12),

(2) 2001 : IFACE in input data #02 is not on the bottom boundary of a partition in the z-direction and

(3) 2222 : The input fixed source for the group 1 is zero including the secondary gamma rays source.

5. Concluding Remarks

Four gamma rays transport codes in the radiation transport code system BERMUDA have been developed for one-, two- and three-dimensional typical geometries. To solve the transport equation numerically, the deterministic direct integration method was adopted in a multigroup model, same as in the neutron transport codes reported in Part I. The Legendre polynomial expansion method was not used in representing the strong anisotropy of gamma rays angular flux and also in calculating numerically the Compton scattering kernel.

The fine energy grid method dividing an energy group into ten fine groups was also applied as in the neutron codes as well as the other methods such as the coarse mesh rebalance of photons. Description on these common methods is in Part I (Reference 1) and has not been repeated in the present report.

A [neutron]-[gamma rays] succeeding calculation has also been possible by connecting the two calculations with job control languages and disk storages of neutron flux.

In course of testing the BERMUDA-2DG code, an error was found in the BERMUDA-2DN code in the thermal energy group neutron calculation. The error was common in BERMUDA-2DN-S16 and BERMUDA-3DN. Now the error has been corrected in these three neutron codes.

Containing the revised neutron codes, the source programs of the following eight transport codes:

(1) BERMUDA-1DN,
(2) BERMUDA-2DN,
(3) BERMUDA-2DN-S16,
(4) BERMUDA-3DN,
(5) BERMUDA-1DG,
(6) BERMUDA-2DG,
(7) BERMUDA-2DG-S16 and
(8) BERMUDA-3DG

will be available to the public through the Code Center of the JAERI (acted now by the Nuclear Energy Data Center (NEDAC)) within 1993.

Part Ⅲ of the present report will be published after improvements of adjoint neutron transport codes in the BERMUDA code system.

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