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A COMPUTER CODE FOR CALCULATING RADIATION SOURCES AND ANALYZING NUCLIDE TRANSMUTATIONS

May 1979

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ORIGEN-JR:

A Computer Code for Calculating Radiation Sources and Analyzing Nuclide Transmutations

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(Received April 9, 1979)

A computer code for calculating radiation sources and analyzing nuclide transmutations has been developed on the basis of the familiar code ORIGEN for reliable shielding calculations of spent fuel cask, fuel reprocessing plant, etc. Energy spectra of neutron sources in spontaneous fissions and (α,n) reactions are available in the code. Angular dependent (α,n) reaction cross sections of eight nuclides (^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O, ^{19}F) are calculated by using the statistical model and compiled as an (α,n) data library. In addition to spectrum indeces adopted in the ORIGEN code, one-group cross sections for each reaction can be used to treat precisely the burnup conditions in a reactor core. Neutron and gamma-ray source data are generated in the same format as in shielding codes QAD-P5, ANISN and DOT-III.

Keywords: Computer Code, Source Evaluation, Nuclide Transmutation, Neutron Source, Gamma-Ray Source, (α,n) Reaction, Light Nuclide, Spent Fuel, One-Group Cross Section, Shielding Calculation, Neutron Spectra, Gamma-Ray Spectra.

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ORIGEN－JR：
同位体元素の生成消滅解析及び放射線源計算コード

日本原子力研究所東海研究所原子炉工学部
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（1979年4月9日受理）

使用済燃料などの輸送容器，再処理工程における線源の評価コードを開発した。同位体元素の生成，消滅計算はORIGENで行なっている。遮蔽詳細設計に必要な中性子エネルギースペクトルについては，自発核分裂中性子源および任意のアクチニド核種と軽元素との（α，n）反応による寄与が計算できる。そのため角度依存（α，n）断面積は，統計模型を用いた計算より8核種（^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O, ^{19}F）についてデータライブリーを作成した。ORIGENで用いられている炉内中性子スペクトル指標の他に，各反応別の一群断面積の使用を可能として，より正確な燃焼条件を取扱える。遮蔽計算コードQAD－P5，ANISN－JR，DOT－Ⅲの線源入力型式に一致した線源データを与えることが可能である。

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1. Introduction

A reliable evaluation of radiation source emitted from spent fuel is required for shielding calculation of transport cask and fuel reprocessing facility to estimate the occupational exposure precisely. Usually, radio-active nuclide concentration of spent fuel has been calculated by using such zero-dimensional burn-up codes with one-group approximation as ORIGEN[1], DCHAIN[2] and PURSE[3] which solve numerically an equation of nuclear transmutation. Most of these codes have a main purpose to calculate nuclide concentration but not to obtain the energy spectrum of source neutron emitted from spent fuel. Therefore, any codes of these are insufficient to obtain the source condition with energy information of neutrons required for a reliable shielding estimation.

These codes have the data library in different formats. However, calculations are performed with the data of decay constants, and neutron induced cross sections collapsed into one-energy group. In any codes, the neutron energy spectrum dependency of one-group cross section has not been considered sufficiently so that the results calculated by these codes could not be adopted generally for the evaluation of radiation source emitted from spent fuel.

One-group cross sections used for the calculation have to be the effective values and to be available in the code system.

Number of neutrons emitted from spent fuels depend on the amount of spontaneous fissions of actinides and (α,n) reactions of light elements such as ^{9}B, ^{13}C, ^{17}O, ^{18}O, and ^{19}F, where α-particles emitted from the actinides increase as the fuel burn-up increases. However, the contribution of (α,n) reactions to the neutron emission rate is calculated by an empirical formula of $^{238}PuO_2$ in ORIGEN, so that neutron due to other nuclides can not be evaluated reliablly.

In order to develop a new code without any problems mentioned above for calculating the source intensity of spent fuels, the ORIGEN was employed as a basis because of the availability of its library form. Newly developed code of ORIGEN-JR has a high ability for the treatment of nuclear transmutations and radioactive sources because of i) replacement of the neutron induced cross section by the effective value generated in the code, ii) incorporation of (α,n) reactions in a general form and iii) incorporation of the neutron energy spectrum calculation in connection with spontaneous fission and (α,n) reactions. Furthermore, ORIGEN-JR can

be used as a computational module of RADHEAT-V3[21] code system, and neutron and gamma-ray sources generated by this code can directly be applied to shielding calculation codes such as ANISN, DOT-III and QAD-P5.

Chapter 2 consists of explanation of the modified methods and systematization needed for use of this code. In Chapter 3, we describe the input instructions.

2. Main Features of ORIGEN-JR

2.1 One-Group Cross Section

In the ORIGEN code, one-group cross sections are obtained from three-group cross sections, which are 2200 m/sec., resonance internal and fission spectrum averaged cross sections with spectrum indeces, THERM, RES, and FAST respectively. These indeces, definitions of which are shown in Table 1, are used as weighting indeces of energy spectrum decided by a given reactor type. However, the energy ranges of these three groups are so wide that an accurate collapsing of the cross sections is generally unattainable. Furthermore, the energy spectrum in the fuel region depends generally on the chemical composition and geometrical configuration, operational condition and irradiation time. In ORIGEN-JR, the routine which processes the one-group cross sections is modified so as to be able to use spatial dependent neutron spectra in a given fuel region by considering the chemical composition and the geometrical configuration. That is, fine group cross sections for each element of the core region are, at first, produced by using the RADHEAT-V3[21] system. Secondly, the spatial dependent neutron spectra in the core region are calculated by using the fine group cross sections by a transport code. Then, the fine group cross sections for each reaction shown in Table 2 are collapsed into one-group cross sections by using the spectra.

A schematic flow of the process is shown in Fig. 1. By applying this procedure for each time step of the operation, the time dependent one-group cross sections are given. Updatings of these one-group cross sections are performed in by the subroutine NUDATA. The nuclide to be updated are assigned by subroutine LIBRY. If the one-group cross sections given in Table 2 can not be obtained for any nuclides, the original values in ORIGEN can be put by simple user's assign.

Table 1 Definitions of three spectrum indeces used in ORIGEN

THERM	;	ratio of the neutron reaction cross section rate for a 1/v absorber with a population of neutrons that has a Maxwell-Boltzmann distribution of energies at absolute temperature, T, to the reaction rate with 2200 m/sec. neutrons. (i.e., $\frac{\sqrt{\pi}}{2}\sqrt{\frac{T_o}{T}}$, T_o = 293.16 °K)
RES	;	ratio of the resonance flux per unit lethargy to the thermal neutron flux. Resonance flux energy boundaries are 0.5 eV and 1 MeV.
FAST	;	1.45 times the ratio of flux above 1 MeV to the thermal neutron flux.

Table 2 Reaction types of one-group cross sections

Element	Reaction type
Light element	(n,γ), (n,p), (n,α), (n,2n), (n,3n)
Actinide element	(n,γ), (n,f), (n,2n), (n,3n)
Fission products	(n,γ)

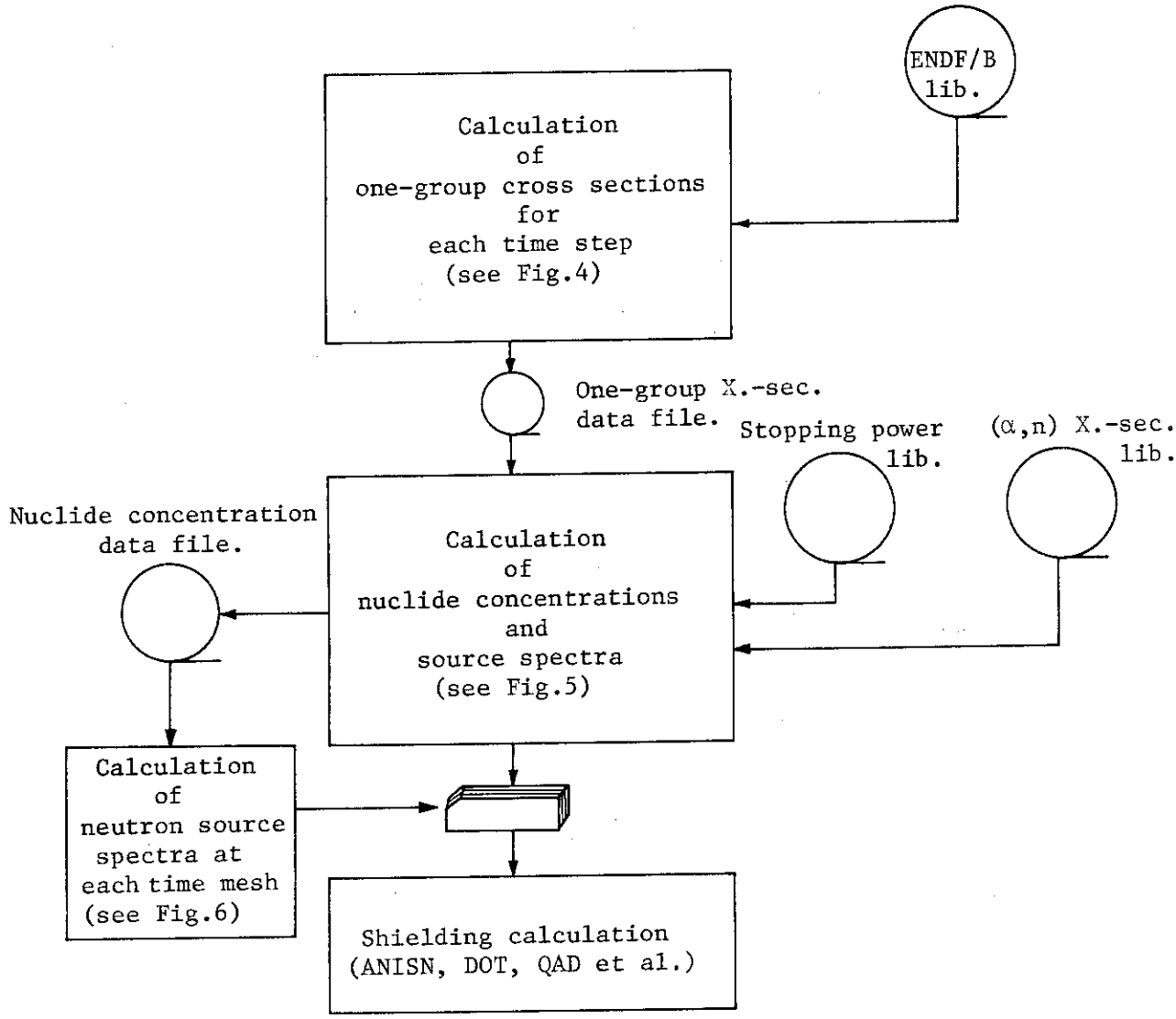

Fig.1 Schematic diagram of ORIGEN-JR system

2.2 Neutron Spectrum due to (α,n) Reaction

In the original ORIGEN, number of neutrons emitted from (α,n) reactions is calculated by using the empirical formula described below.

$$n = 1.0 \times 10^{-10} E_\alpha^{3.65}, \tag{2.1}$$

where n is the intensity of emitted neutrons by (α,n) reactions (n/sec) and E_α is the α-particle energy emitted by the actinide nuclide (MeV). This formula is based on the results given by a measurement of (α,n) reactions of $^{238}PuO_2$. Therefore, the results calculated by using this formula depend neither on a variation of the ratio of ^{238}Pu to ^{18}O concentration nor other chemical composition, that is, carbide, nitride and fluoride of actinides.

The method to calculate the neutron source intensity due to (α,n) reactions in ORIGEN-JR is extensively revised by taking into consideration all the informations related to the neutron energy spectrum. Emitted neutron spectra of (α,n) reactions are calculated by the following method. The (α,n) reaction rate per unit time and unit volume is given by

$$\Delta N = n_T \sigma_T(E_\alpha) \cdot \phi(E_\alpha) \Delta E_\alpha \ . \tag{2.2}$$

where E_α is α-particle energy in L,M.S. (laboratory of mass system), n_T is number density of target nuclei, σ_T is total cross section of (α,n) reaction, and ϕ is scalar flux of α-particles. The emitted neutron energy E_n in L.M.S. has the following connection with E_α.

$$E_n = E_n^{\,0} + \frac{m_n m_\alpha}{(m_\alpha + m_T)^2} E_\alpha + 2 \frac{\sqrt{m_n m_\alpha}}{m_\alpha + m_T} (E_n^{\,0} + E_\alpha)^{1/2} \cos\theta \ , \tag{2.3}$$

where $$E_n^{\,0} = \frac{m_F}{m_F + m_n} \left(\frac{m_T}{m_F + m_\alpha} E_\alpha + Q \right) \ , \tag{2.4}$$

m_n, m_α, m_T, m_F are masses of neutron, α-particle, target nucleus, and residual nucleus, respectively. In addition, θ is scattering angle in C.M.S. (center of mass system) and Q is reaction energy of residual nucleus, that is

$$Q = Q_o - E_\ell \ , \tag{2.5}$$

where Q_o is so called Q-value and E_ℓ is the energy for the level, ℓ of residual nucleus. The energy level of target nucleus is assumed to be the ground state.

The α-particle energy spectrum is approximated as follows:

$$\phi(E_\alpha) \doteqdot \sum_{i>E_\alpha} n_{\alpha i}/(dE/ds)E_\alpha \ , \tag{2.6}$$

where

$$(dE/ds)E_\alpha = \sum_j \rho_j (dE/dm_j)E_\alpha \ , \tag{2.7}$$

$n_{\alpha i}$ is number of α-particles emitted by actinide nuclide per unit time, (dE/ds) is stopping power which is given approximately by Eq. (2.7), ρ_j is density of nuclide, j, and (dE/dm_j) is energy loss per (mass/area).

Then neutrons emitted within the energy group i ($E_{i+1} \leq E \leq E_i$) per unit volume and unit time are described as

$$\int_{E_{i+1}}^{E_i} N(E)dE = 2\pi \sum_{\{T,Q\}} n_T \sum_j \Delta E_\alpha^j \int_{\cos\theta_1}^{\cos\theta_2} \phi(E_\alpha^j) \frac{d\sigma_T^Q(E_\alpha^j,\theta)}{d\Omega} d(\cos\theta) \ . \tag{2.8}$$

If the (α,n) differential cross section is expressed by the following Legendre expansion:

$$\frac{d\sigma_T(E,\theta)}{d\Omega} = \sum_\ell f_\ell P_\ell(\cos\theta) \ , \tag{2.9}$$

it follows from Eqs. (2.8) and (2.9) that

$$\int_{E_{i+1}}^{E_i} N(E)dE = 2\pi \sum_{\{T,Q\}} n_T \sum_j \Delta E_\alpha^j \cdot \phi(E_\alpha^j) \sum_\ell f_\ell \int_{\mu_1}^{\mu_2} P_\ell(\mu)d\mu, \tag{2.10}$$

where $\mu = \cos\theta$.

In ORIGEN-JR code, the differential cross sections of (α,n) reactions are stored in the form of Legendre coefficients, f_ℓ in the (α,n) deta library. Target nuclides contained in the library are ^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O, and ^{19}F. The energy levels of residual nuclei are considered up to forth excitation level. Neutron energy groups are 200 from 14.9 MeV to 0.1 MeV with a lethargy width of 0.025. The α-particle energy is calculated for 100 points from 10 MeV to 1 MeV with an equal spacing of energy. The (α,n) differential cross section has a complicate structure so that it will be necessary to use at least 100 groups in this code. Large number of group are needed when more precise spectrum is required. Moreover, energy levels of residual nucleus are required to be more than 5.

The stopping power library has the data[12] for 58 materials and the

subroutine SPOWER reads this library and interpolates the values by energy. The subroutine GROUP processes these procedures of (α,n) reactions. The Q-values and residual nucleus excitation levels in the (α,n) library are quoted from Nuclear Data Sheets.[5)~11)]

Detailed description of data library is given in Appendix E and method of calculations is given in the reference 13.

2.3 Neutron Spectrum Emitted from Spontaneous Fission

The ORIGEN code gives no information of spontaneous fission energy spectrum emitted by actinide. The ORIGEN-JR is revised to be able to calculate the energy spectrum of Maxwellian ENDF/B type. This procedure is followed in the subroutine GROUP. The energy spectrum of Maxwellian ENDF/B type is follows:

$$\phi_s(E) = \frac{2}{T(\pi T)^{1/2}} E^{1/2}\exp(-E/T) , \tag{2.11}$$

where T is given by Terrell's formula[1)]:

$$T = 0.5 + 0.43 \sqrt{(\bar{\nu}+1)} , \tag{2.12}$$

in which $\bar{\nu}$ is average neutron number per fission given by

$$\bar{\nu} = 2.84 + 0.1225\ (A-244) , \tag{2.13}$$

where A is atomic number of actinide nuclide.

Then, neutrons emitted in the energy group $i(E_{i+1} \leq E \leq E_i)$ are written as follows:

$$S_i = \int_{E_{i+1}}^{E_i} \phi_s(E)dE = \frac{2}{\sqrt{\pi}} \{\eta_{i+1}^{1/2} e^{-\eta_{i+1}} - \eta_i e^{-\eta_i} + \mathrm{erf}(\xi_i) - \mathrm{erf}(\xi_{i+1})\}, \tag{2.14}$$

where
$$\left.\begin{aligned} &\eta = E/T , \\ &\xi = \eta^{1/2}, \\ &\mathrm{erf}(x) = \int_0^x e^{-t^2} dt. \end{aligned}\right\} \tag{2.15}$$

Clearly, Eq. (2.14) is normalized to unity.

2.4 Energy Group Boundary for Gamma Rays

The ORIGEN calculates γ-ray spectrum emitted from light elements, fission products and actinides in the forms 12, 12, and 18 groups, respectivley. However, a uniform group structure is necessary used at the stage of shielding calculations so that they are rearranged to the group structure of EURLIB 20 groups. The transformation procedure is to allocate proportionally by lethargy as shown in Fig. 2 and Table 3.

Table 3 Typical transformation formula of energy group structure

Group	Transformation formula
k	$I_1 \cdot \frac{\ln(E_j/E_{j+1})}{\ln(E_i/E_{i+1})}$
k+1	$I_1 \cdot \frac{\ln(E_{j+1}/E_{i+1})}{\ln(E_i/E_{i+1})} + I_3 \cdot \frac{\ln(E_{i+1}/E_{j+2})}{\ln(E_{i+1}/E_{i+2})}$
k+2	$I_3 \cdot \frac{\ln(E_{j+2}/E_{j+3})}{\ln(E_{i+1}/E_{i+2})}$
k+3	$I_3 \cdot \frac{\ln(E_{j+3}/E_{i+2})}{\ln(E_{i+1}/E_{i+2})} + I_2 \cdot \frac{\ln(E_{i+2}/E_{j+4})}{\ln(E_{i+2}/E_{i+3})}$

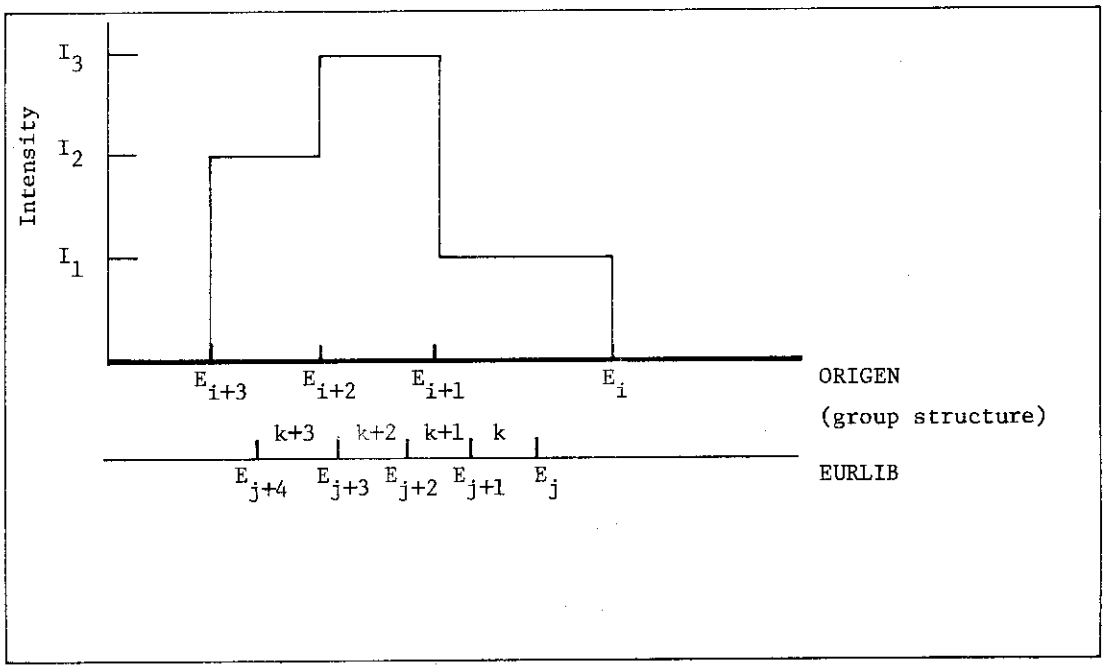

Fig.2 Typical transformation of energy group structure

2.5 Preparations of Source Data for Shield Calculation Codes

The ORIGEN-JR has been fitted to input formats of various shielding calculation codes. The available formats are for QAD-P5,[14] ANISN,[15] DOT[16] and user's one described in 2.5.4.

2.5.1 QAD-P5[14]

If it is assigned IO=0 in card I (see Chapter 3), the output format is as follows;

card 1 ; identification card.
card 2 ; ibid.
card 3 ; ALLG (E9.2)
card 4 ; EX(I), I=1,20 (8E9.2)
card 5 ; identification card.
card 6 ; ALLN (E9.2)

In these cards, ALLG and ALLN are source intensity of γ-rays and neutrons, respectively, in units of (particles/sec.). The EX is γ-ray energy distribution normalized to unity. Energy group boundaries are the same as for EURLIB (see reference 20).

2.5.2 ANISN[15]

If it is assigned IO=1 in card I, the output format takes the ANISN free FIDO form of 17* array. Collapsing by energy is available when IEQ of card I is a positive number. IEQ is the total number of few-groups and few-group numbers for each multigroup are assigned by IQB of card J given below.

Example: In the case of shielding configuration shown in Fig. 3, input values of I and J cards are as follows;

card I ; IO=1, IM=60, IIM=1, IIS=10, V=100.0, and IEQ=20
card J ; (IQB(I), I=1, 120) are
1 1 1 1 1 2 2 2 2 2 . . . . .
. . . 19 19 19 19 19 20 20 20 20 20.

Note; original 120 group structure is constructed by DLC-II type 100 groups of neutrons and EURIB type 20 groups of γ-rays.

The output cards are as follows;

card 1 ; identification card.

card 2 ; 17**

card 3 ; 10R (source intensity of group 1) 50R0.0

⋮

card 23; 10R (source intensity of group 20) 50R0.0

card 24; T

Note; units of these intensities are (particles/cm^3·sec.).

2.5.3 DOT[16)]

If it is assigned IO=3 in card I, the output takes the DOT free FIDO form of 17* array. Few group parameters of card J should be given and collapsing manner is the same as the example described in Section 2.5.2. In this case, parameters IM, IIM, and IIS have no meaning for the output because of the assumption that energy and spatial distributions are separable. Output cards have only the information of energy distribution. Then the spatial distribution must be assigned by user in another 17* array.

In this case, output form are as follows;

card 1 ; identification card

card 2 ; 17**

card 3 ; (source intensity of group 1)

⋮

card N ; (source intensity of last group)

card N+1; T

Units of these intensities are (particles/cm^3·sec.).

2.5.4 User's format

This format is determined for convenience' sake to preserve the result of calculation or to revise it for another shielding code developed by user. The format is as follows;

(FX(I), I=1, 120) (8E10.3)

Units of these values are (particles/sec.).

2.6 Necessity of Systematization

In the case that it is required a precise source evaluation of spent fuels, burnup calculation must be done carefully by using one-group cross

sections produced by energy spectrum weighting. Calculations of neutron spectra may be performed by each adequate time step because concentrations of nuclides in the core region change with irradiation. Moreover, neutron spectrum emitted by spontaneous fission and (α,n) reactions and γ-ray spectrum must be calculated in an energy group structure of shielding calculation. To perform a series of these processes effectively, it is necessary to systematize these codes rather than using independently. The ORIGEN-JR is therefore produced to respond this request. The schematic diagram of this system is shown in Figs. 1 and 4∿6.

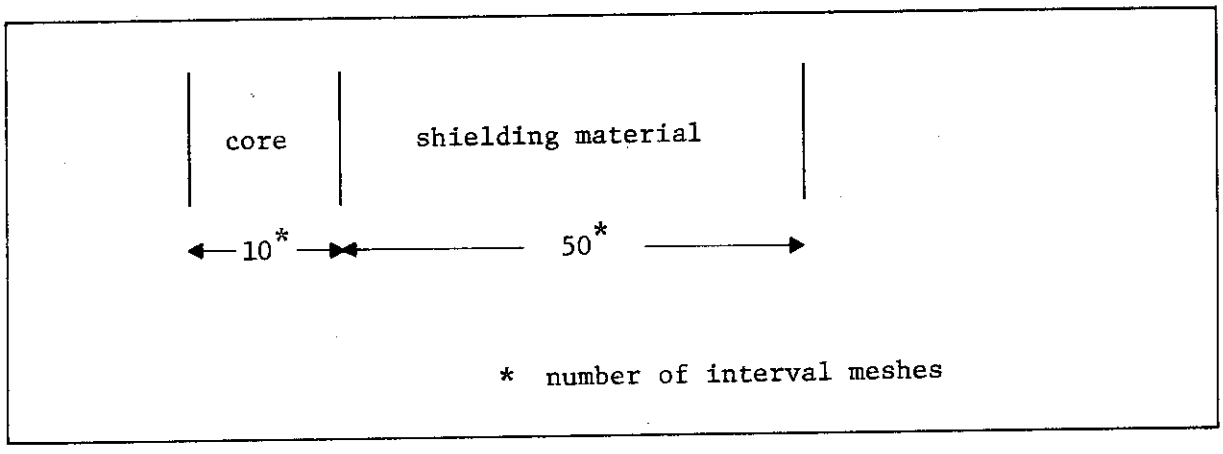

Fig.3 Typical configulation† of shielding calculation

† Number of energy groups is 20 and collapsing are done every five groups. Core volume is 100 cm^3.

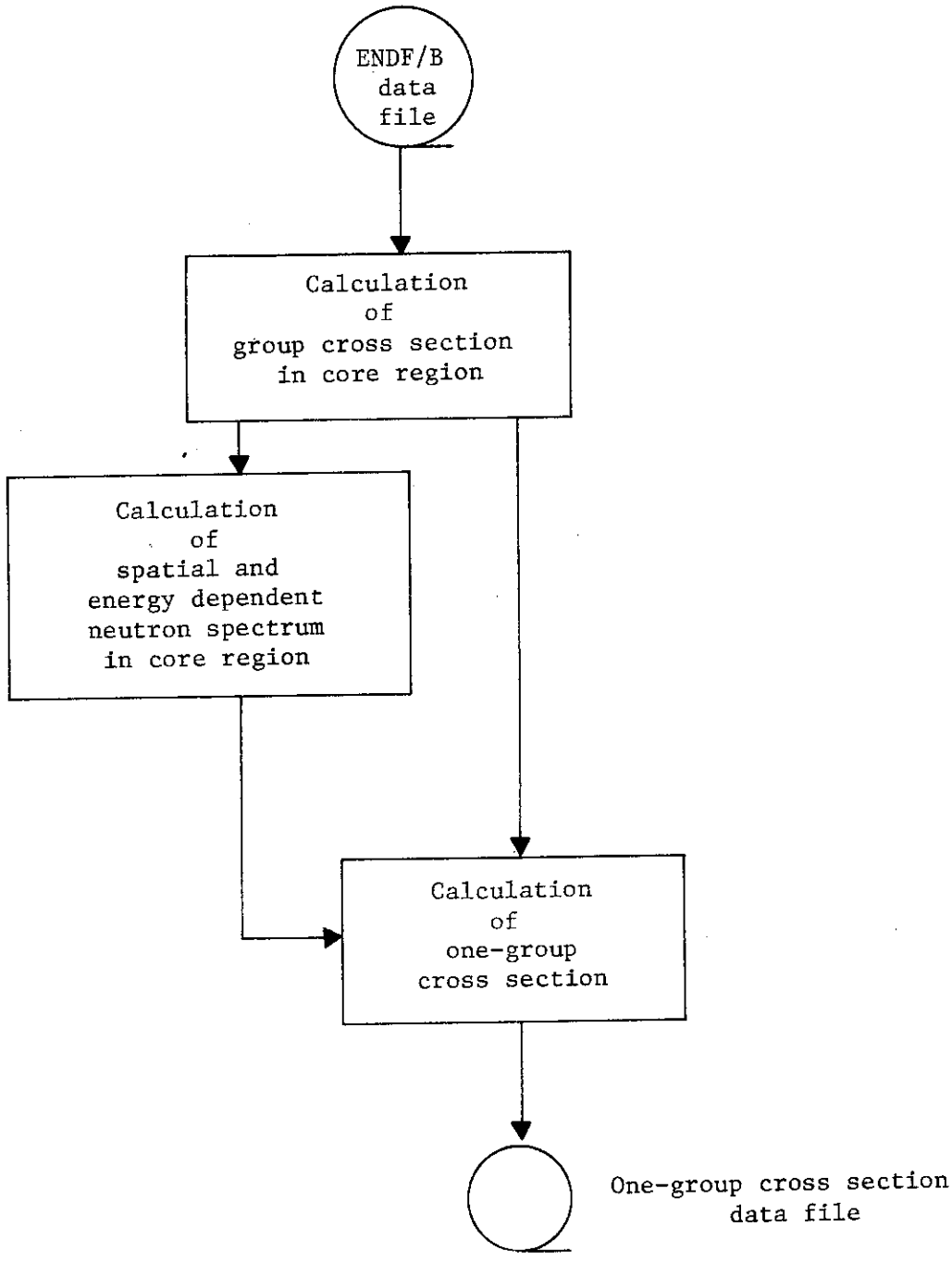

Fig.4 Schematic diagram of one-group X.-sec. calculation

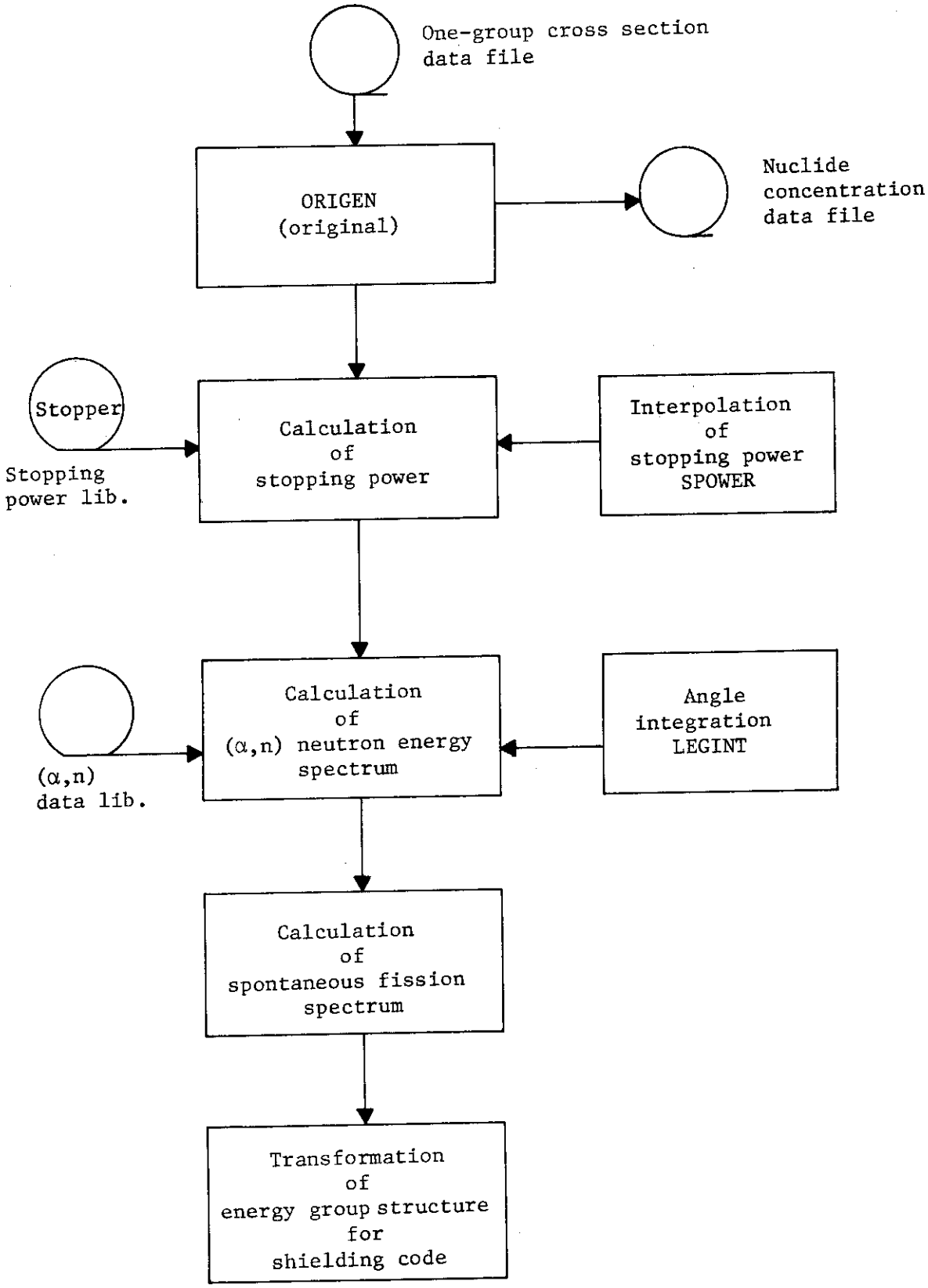

Fig.5 Schematic diagram of ORIGEN-JR

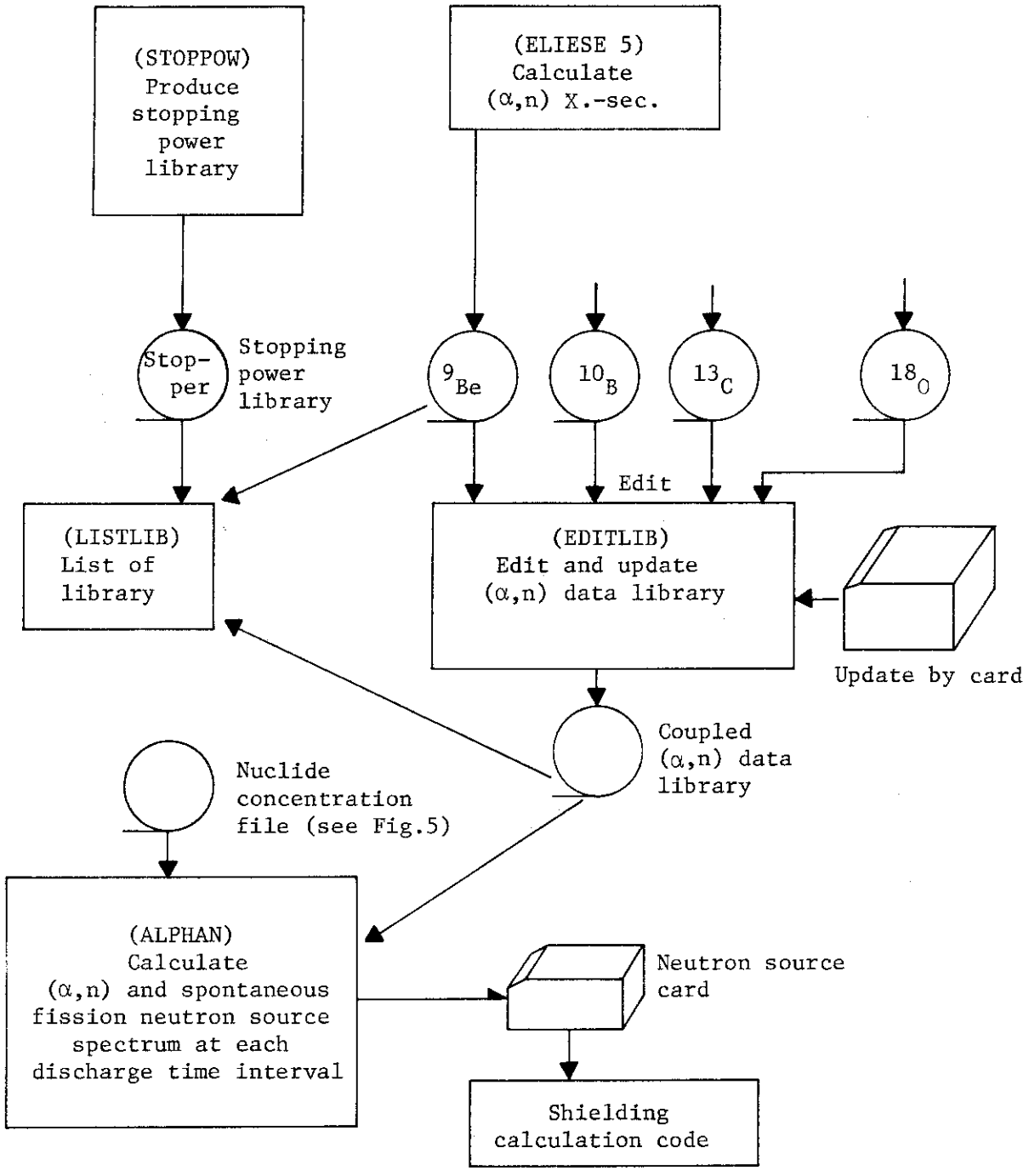

Fig.6 Schematic diagram of utility codes

3. Input Instruction

CARD A. Title card. Format (18A4, I3, I3)

TITLE ; title,

NLIBE ; identification number of library data to be read,
= 1 - HTGR,
2 - LWR,
3 - LMFBR,
4 - MSBR.

NTOP ; option for one-group cross section data to be updated,
= - N - read from file assigned logical unit N,
0 - no update,
N - number of update cards.
Positive number assigns to read from cards.

CARD B. Control data for library. Format (4F10.5, 7I2)

THERM ; spectrum index for thermal flux,

RES ; spectrum index for resonance flux,

FAST ; spectrum index for fast flux.

Definitions of the parameters mentioned above are described in Table 2.1.

ERR ; truncation error limit (1.0×10^{-25} recommended),

NMO ; month
NDAY ; day
NYR ; year
} when calculation is performed.

MPCTAB ≠ 0 - print RCG-value table for water and air,
= 0 - do not print.

INPT ≠ 0 - update photon data,
= 0 - do not update.

IR ≠ 0 - print transition matrix,
= 0 - do not print.

LPU = N - number of actinide data to be updated ($\leq$11),
= 0 - do not update.

CARD C. Output option for print table. Format (40I2)

1 - do not print,

0 - print,

LMBWR1 ; neutron library data for light elements,
LIBWR2 ; neutron library data for actinide elements,
LIBWR3 ; neutron library data for fission products,
LIBWR4 ; library data for RCG,
LIBWR5 ; γ-ray library data for light elements,
LIBWR6 ; γ-ray library data for actinide elements
LIBWR7 ; γ-ray library data for fission products,

NWROU1 ; calculated results for light elements,
NWROU2 ; calculated results for actinides,
NWROU3 ; calculated results for fission products,
NWROU4 ; not used,
NWROU5 ; not used,

NWRTA1 ; unit of table, g-atom
NWRTA2 ; unit of table, g
NWRTA3 ; unit of table, C_i
NWRTA4 ; unit of table, watt (thermal)
NWRTA5 ; unit of table, watt (γ-ray)
NWRTA6 ; unit of table, RCG (air)
NWRTA7 ; unit of table. RCG (water)

CARD D. One group cross section data to be updated. Format (I7, 6E12.4)
(NTOP>0)

MAT ; material identification number to be updated,
FIS ; fission reaction cross section (barns),
SINP ; (n,p) reaction cross section (barns),
SINA ; (n,α) reaction cross section (barns),
SING ; (n,γ) reaction cross section (barns),
SIN2N ; (n,2n) reaction cross section (barns),
SIN3N ; (n,3n) reaction cross section (barns).

If these values equal to -1.0, one group cross sections are produced from the ORIGEN original library.

CARD E. Material identification number of actinides to be updated.
Format (I6, 10I7) (LPU>0)

(NEWCX(I), I=1, LPU); material identification number of actinides to be updated.

CARD F. Data for actinides to be updated. (7X, 2F9.2, F5.3, 4F9.2, F4.3, F9.2, I1) (LPU>0)

SIGNG ; (n,γ) cross section for thermal energy group (barns),

FING ; (n,γ) cross section for resonance energy group (barns),

FNG1 ; fraction of (n,γ) absorption that results in an excited nuclear state of the product nuclide,

SIGF ; (n,f) cross section for thermal energy group (barns),

SIF ; (n,f) cross section for resonance energy group (barns),

SIGFF ; (n,f) cross section for fast energy group (barns),

SIGN2N ; (n,2n) cross section for fast energy group (barns),

FN2N1 ; fraction of (n,2n) reaction that result in the formation of a product nuclide in an excited nuclear state,

SIGN3N ; (n,3n) cross section for fast energy group (barns),

IT ; an index indicating the reactor spectrum with which cross sections have been averaged.

CARD G. Data for photons to be updated. Format (I6, 12F6.4, I2) (INPT≠0)

NUCLID ; nuclide identification number,

GFRAC(1); photon release data for energy group 1,

GFRAC(12); photon release data for energy group 12,

NPHOT ; not used.

CARD H. Control data for calculation. Format (16I5)

MMN ; number of mesh intervals for irradiation time (≤10),

MOUT ; number of mesh intervals for total period (irradiation + cooling) (≤10),

NOBLEND ; number of materials to be blended (≤10),

INDEX ; input index for power or flux,
= 0 - power
1 - flux.

NTABLE ; print only essential results,
= 0 - no,
≠ 0 - yes.

MSTAR ; interval number applied to cut-off value (see Q card),

NGO ; connection condition for next calculation,
=-N - different initial condition and same nuclear data (next start is from card H),
0 - different initial condition and different nuclear data (next start is from card A),
1 - continued condition and same nuclear data (next start is from card X),
10 - continued condition and different nuclear data (next start is from card X).

MPROS ; number of continuous chemical processing (≤8),
= 0 - do not process.

MFEED ; option for continuous fuel charging,
= 0 - do not operate,
≠ 0 - operate.

JTO ; option for print table of cooling interval,
= 0 - print all table,
1 - do not print,
2 - print for selected table (≤63) (see card K).

NOPT ; Interval number of time for calculation of source spectra.

If NOPT=-1 is entered, source spectra at the initial time period are calculated.

CARD I. Option for output of punched card. Format (4I5, 2X, F8.4, I5) (NOPT≠0) (detailed informations are described in Section 2.5)

IO ; codes for shelding calculation,
= 0 QAD-P5,
1 ANISN,
2 DOT-III,

5 output in user's format,
10 QAD-P5 and user's format,
11 ANISN and user's format,
12 DOT-III and user's format.

IM ; number of total mesh intervals (IO=1 or 11),

IIM ; first interval number of source region (IO=1 or 11),

IIS ; number of source mesh intervals (IO=1 or 11),

V ; volume of source region (cm^3),

IEQ ; number of few-groups (IO=1, 2, 11 or 12).

CARD J. Few-group parameters. Format (20I4) (IEQ≠0)

(IQB(I),I=1,120); few-group numbers for each multigroup,
1≤I≤100 are neutron energy groups (DLC-II type),
101≤I≤120 are γ-ray energy groups (EURLIB type).

CARD K. Additional options. Format (3X,7(7X,3I1)) (JTO=2)

This card controls selection of output table.

(NTO(I),I=1,63) ; 1 - print,
0 - do not print.

I= 1 - g-atom ; light elements by each time step,
2 - g-atom ; light nuclides by each time step,
3 - g-atom ; light nuclides and elements by every 2 time steps,
4 - gram ; sequence is same as above,
5 - gram ;
6 - gram ;
7 - C_i ; ibid.,
8 - C_i ;
9 - C_i ;
10 - thermal power; ibid.,
11 - thermal power;
12 - thermal power;
13 - γ-power ; ibid.,
14 - γ-power ;
15 - γ-power ;
16 - RCG (air) ; ibid.,
17 - RCG (air) ;

18 - RCG (air) ;
19 - RCG (water) ; ibid.,
20 - RCG (water) ;
21 - RCG (water) ;
22∿42 - sequence is same as above; sequence is same as above but for actinide materials,
43∿63 - ibid., ; sequence is same as above but for fission products.

CARD L. Title. Format (20A4)

This title is printed on each output table.

CARD M. Power of each irradiation time period. Format (10E8.2) (INDEX=0)

POWER(I), I=1, MMN ; specific thermal power at each irradiation time period (I), (MW/unit of fuel)

There may be periods of zero power; however, there may not be two consecutive zero power intervals, and the final irradiation period may not have zero power.

CARD N. Flux of each irradiation time period. Format (10E8.2) (INDEX=1)

FLUX(I), I=1, MMN ; thermal neutron flux at irradiation time period ($n/cm^2 \cdot sec.$) or the total neutron flux for a fast reactor (inhibit conditions are same as above).

Cards of type M or N are included only if MMN is greater than zero.

CARD O. Time mesh intervals. Format (10E8.2)

T(I), I=1, MOUT ; elapsed time since the beginning of the calculation. (measured in term of TUNIT)

CARD P. Title and unit of time. Format (10A4, F7.0, A3)

BASIS ; title of the unit of fuel for output table (e.g., "Ton of U"),

TCONST ; a factor to convert input values of T(I) into seconds (e.g., if time unit is a day, TCONST is 24 × 60 × 60 =

86400),

TUNIT ; an alphameric designation for input units of T(I) (e.g., "DAY" for days).

CARD Q. Threshold value. Format (7E10.3)

CUTOFF(MS) ; a threshold value to output summary tables. Any isotopes whose value in the time period MSTAR is less than this value will be omitted from the summary table of property MS.

MS =			
1	- g-atom table	(recommended 0.001),
2	- gram table	(recommended 0.001),
3	- Curie table	(recommended 0.001),
4	- $\beta + \gamma$ power table	(recommended 0.001),
5	- γ-power table	(recommended 0.001),
6	- relative inhalation hazard	(recommended 1.0),
7	- relative ingestion hazard	(recommended 1.0).

CARD R. Compositions of blended fuel. Format (8E10.3) (NOBLND≠0)

FACT(I), I=1, NOBLND ; atom fraction of each material in a calculation for a blended fuel.

CARD S. Initial concentrations. Format (5(I6, E9.2),I5)

INUCL(I) ; nuclide identification number,

XCOMP(I) ; initial concentration of nuclide INUCL (expressed as g-atoms/unit of fuel),

NEXT ; an indicator giving the type of the five isotopes on the card (thus all five must be of one type).

=		
1	-	isotopes of cladding and structual materials,
2	-	isotopes of heavy metals,
3	-	isotopes of fission products,
4	-	elements of cladding and structual materials.

All cards of this type should be followed by a single blank card.

CARD T. Chemical processing conditions. Format (8(E8.2, I2)) (MPROS>0)

PRATE(I) ; first order removal constant for chemical processing by processing stream I (sec^{-1}),

NOPROS(I) ; number of elements removed by stream I.

CARD U. Atomic number of chemical processing. Format (20I4) (MPROS>0)

(NZPROS(M,N), N=1, NOPROS), M=1, MPROS) ;
atomic number of element N in processing stream M.

CARD V. Feed rate of chemical processing. Format (5(I6, E9.2), I5) (MFEED>0)

INUCL(I) ; definition is same as card K of INUCL,
XCOMP(I) ; continuous feed rate of isotope INUCL,
NEXT ; definition is same as card K of NEXT.

The following cards W1 ∿ W4 are read only if NOPT≠0.
These cards controls calculation of (α,n) and spontaneous fission neutron source spectrum. If NOPT=0, it is no calculation of neutron source spectrum and no output of punched card for shielding calculation.

CARD W1. Control card of calculation for (α,n) reaction. Format (7I5, E12.5) (NOPT≠0)

ID1 ; 1 - output nuclide concentrations to logical unit No.21,
0 - no effect.

ID2 ; 1 - print α-particle energy spectrum by each actinide,
0 - no effect.

ID3 ; 1 - print detailed table,
0 - no effect.

ID4 ; 1 - print neutron source spectrum by each light nuclide,
0 - no effect.

ID5 ; 1 - calculate spontaneous fission neutron source spctrum,
0 - no effect.

ID6 ; 1 - punch source card,
0 - no effect.

ID7 ; 1 - read data of structural nuclide,
0 - no effect.

FT ; conversion factor of unit of concentration.
if FT = 0.0, unit is g-atom/unit of fuel.

The following cards W2 ∿ W4 are only for use of (α,n) neutron calculations.

CARD W2. Nuclide assignments. Format (8I10)

NAE ; number of actinide nuclides to be processed,

NOAE(I),I=1,NAE ; identification number for actinides.

CARD W3. Nuclide assignments. Format (8I10)

NLE ; number of light nuclides to be processed,

NOLE(I),I=1,NLE ; identification number for light nuclides.

In this code the light nuclides are only 8 isotopes. (i.e., ^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O and ^{19}F) If different light nuclides are assigned, it will be no calculation of (α,n) source spectrum.

CARD W4. Nuclide assignments. Format (8I10) (ID7=1)

NME ; number of structural nuclides to be processed,

NOME(I),I=1,NME ; identification number of structural nuclides.

For the above-mentioned input data, the program calculate the isotopic compositions for all MOUT time periods and write the output. After writing the output, the program will either be ready to start a new problem (if NGO>0) or continue the present one (NGO≤0). In the condition of NGO=1 in the card H, the input for the continuation of calculation has the form;

CARD X. Control data for calculation. Format (16I5)

MMN ; same as card H,

MOUT ; ibid.,

NOBLND ; ibid.,

INDEX ; ibid.,

MSUB ; time period in the last calculation considered as the start of the new calculation (also used to indicate that batch chemical processing occurs if the value in negative).

MSTAR ; same as card H,

NGO ; ibid.,

MPROS ; ibid.,

MFEED ; input indicator for continuous feed,

= 0 - no feed,

N - continuous feed at the same rate as for the previous

calculation.

JTO ; same as card H,

NOPT ; ibid..

This card is followed by cards of type I, J, K, L, M, N, O, P or Y, Z (see below), W1 ∿ W4 to complete the input for the continued calculation. This procedure may be repeated as desired. The calculation will stop when a blank card is read in place of a card of type H. When continuing a calculation that was started in a previous set of time periods, a card or type P may be modified to include one additional piece of information.

CARD Y. Title and unit of time. Format (10A4, F7.0, A3, F10.3)

BASIS ; definition is same as card P,

CONST ; ibid.,

TUNIT ; ibid.,

TMO ; the time value of previous calculation defined as initial period of present ones.

In the case of continuous condition, this value is defined as the initial time of present calculation. The unit is given by TUNIT. If TMO≠0, the values of times of card O must be given as the continuous value from the previous calculation. Whereas the case that the time period is defined as a discharge time, the value of TMO is no meaning.

A negative value for the variable MSUB indicates that batch chemical processing is assumed to occur at time T(-MSUB), and that data giving a processing information are required to be read. When MSUB has a negative value, cards of the type Z are expected to follow card Y.

CARD Z. Removed chemical element assignmnet. Format (I6, 4X, E10.3)
(MSUB<0)

LEMENT ; atomic number of a certain chemical element to be removed,

FREPRO ; fraction of the material that remains after processing.

The array FREPFO is initially set equal to 1.0; thus, if no data are read for an element, processing does not affect its concentration. Cards of type Z are expected to be read until a blank card is encountered.

In the condition of NGO = 10 in the card H, the card X is followed by cards of type I, J, K, L, M, N, O, P or Y, Z, A, B, C, D, E, F, G, W1 ∿ W4.

This is all of the card input that is required to perform a variety of calculations with the ORIGEN-JR code.

4. Sample Input

A usage of the ORIGEN-JR is illustrated with a sample problem, in which transmutations of nuclides and radiation source strength are calculated in a BWR core. The conditions of the problem are assumed as follows;

i) operating power : 21.6 MW/ton of heavy metal
ii) irradiation time : 1000 days
iii) cooling time : 150 days
iv) initial charge : shown in Table 4.

Some new functions added into the ORIGEN-JR are applied by the problem of which the input data are shown in Fig. 7, described below.

v) The function to update one-group cross sections is used by the data in the cards from the ID number of 4 to 18, shown in Fig. 7.

vi) The function to calculate the radiation source for shielding calculation codes is used by the data in the cards from the ID number 20 to 26. By using these data, the radiation source cards for the input data of ANISN are directly generated.

vii) The function to calculate the neutron source emitted from the (α,n) reaction is used by the data on the cards from the ID number of 36 to 39.

Table 4 Initial charges in use of the sample problem

Nuclide	Initial charge*
^{16}O	8.176×10^{3}
^{17}O	3.189
^{18}O	1.676×10^{2}
^{235}U	3.772×10^{1}
^{238}U	4.0989×10^{3}
^{239}Pu	3.754×10^{1}
^{240}Pu	1.576×10^{1}
^{241}Pu	8.820
^{242}Pu	3.097

* unit is g-atom/ton of heavy metal

```
                    **********
                    *        *
                    *  INPUT DATA LIST  *
                    *        *
                    **********

    ....*....1....*....2....*....3....*....4....*....5....*....6....*....7....*....8
 1    TEST CALCULATION  CASE OF BWR ( U+PUO2 )                                2 15
 2      0.4274    1.917     1.45      1.0E-25060278
 3   1 1 1 1 1 1 1 0 0 0 0 0 0 0 1 1 1 1 1 0 0 0 0
 4   922350 43.37       -1.0        -1.0        10.21       -1.0
 5   922360 0.1909      -1.0        -1.0        7.164       -1.0
 6   922380 0.0933      -1.0        -1.0        0.8189      0.00567
 7   932370 0.0012      -1.0        -1.0        30.62       0.00116
 8   942380 1.749       -1.0        -1.0        37.87       -1.0
 9   942390 97.7        -1.0        -1.0        54.8        0.00114
10   942400 0.4981      -1.0        -1.0        85.09       -1.0
11   942410 109.3       -1.0        -1.0        36.4        -1.0
12   942420 0.4131      -1.0        -1.0        26.1        -1.0
13   952410 0.8377      -1.0        -1.0        85.0        -1.0
14   952421 453.0       -1.0        -1.0        300.7       -1.0
15   952430 0.0043      -1.0        -1.0        60.73       -1.0
16   962420 0.3067      -1.0        -1.0        5.586       -1.0
17   962430 93.89       -1.0        -1.0        28.68       -1.0
18   962440 0.4571      -1.0        -1.0        20.8        -1.0
19      9   10    0    0    1    1    1    0    0    0   10
20      1   50    1   10    10.0      24
21     1   1   1   1   1   2   2   2   2   2   3   3   3   3   3   4   4   4   4   4
22     5   5   5   5   5   6   6   6   6   6   7   7   7   7   7   8   8   8   8   8
23     9   9   9   9   9  10  10  10  10  10  11  11  11  11  11  12  12  12  12  12
24    13  13  13  13  13  14  14  14  14  14  15  15  15  15  15  16  16  16  16  16
25    17  17  17  17  17  18  18  18  18  18  19  19  19  19  19  20  20  20  20  20
26    21  21  21  21  21  22  22  22  22  22  23  23  23  23  23  24  24  24  24  24
27    *  TEST CALCULATION CASE OF BWR ( U+PUO2 )
28  21.6     21.6     21.6     21.6     21.6     21.6     21.6     21.6     21.6
29   10.0    50.0     100.0    200.0    300.0    400.0    600.0    800.0    1000.0   1150.0
30            GRAM-ATOM /TON                    86400.0DAY
31  0.001     0.001     0.001     0.001     0.001     1.0       1.0
32   801608.1760E+3 801703.189     801801.6760E+2                                    1
33  92235037.72    9223804098.9   94239037.54    94240015.76    9424108.82         2
34  9424203.097                                                                     2
35
36      1    1    1    1    1    1    1 0.0
37           7    942380    942390    942400    942410    942420    962420    962440
38           2     80170     80180
39           2     80160    922380
    ....*....1....*....2....*....3....*....4....*....5....*....6....*....7....*....8

*** INPUT DATA END ***
```

Fig. 7 A sample input data for ORIGEN-JR

Acknowledgment

The authors wish to acknowledge Dr. S. Igarasi, Division of Physics, JAERI, for his unfailing advices in making the subroutines which calculate (α,n) reaction cross section. They also wish to thank Dr. T. Asaoka for a critical reading of the manuscript.

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Acknowledgment

The authors wish to acknowledge Dr. S. Igarasi, Division of Physics, JAERI, for his unfailing advices in making the subroutines which calculate (α,n) reaction cross section. They also wish to thank Dr. T. Asaoka for a critical reading of the manuscript.

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Appendix A Mathematical Method used in ORIGEN

The ORIGEN uses the matrix exponential method[17] to solve the equations of radioactive growth and decay for large numbers of nuclides. The formula for concentrations of each nuclide in the neutron flield is described as follows:

$$\frac{dX_i}{dt} = \sum_{j=1}^{N} \ell_{ij}\lambda_j X_j + \bar{\phi}\sum_{k=1}^{N} f_{ik}\sigma_k X_k - (\lambda_i+\bar{\phi}\sigma_i)X_i, \quad (i=1....N) \qquad (A.1)$$

where X_i is the atomic concentration of nuclide i, λ_i is the disintegration constant, and ℓ_{ij} and f_{ik} are ratios of disintegration and production of other nuclides which lead to the generation of nuclide i. The $\bar{\phi}$ is the neutron flux averaged over space and energy, which is assumed constant over period of a short time interval, and σ is the averaged neutron absorption cross section.

A matrix representation of Eq. (A.1) and its solution are expressed as follows:

$$\frac{dX}{dt} = AX \ , \qquad (A.2)$$

$$X(t) = X(0)\exp(At) \ , \qquad (A.3)$$

where X(0) is the initial atomic density at time = 0. A is the transmutation matrix containing the decay and production coefficients. By applying a Taylor series expansion to Eq. (A.3), we get

$$X(t) = X(0)\ \{I + At + \frac{(At)^2}{2} + ...\}$$

$$= X(0)\sum_{m=0}^{\infty}\frac{(At)^m}{m!} \ . \qquad (A.4)$$

Now, X(t) is expanded as follows:

$$X(t) = \sum_{n=0}^{\infty} C^n \ . \qquad (A.5)$$

Substituting Eq. (A.5) to Eq. (A.4), then the following recursion formula is obtained.

$$C^0 = X(0) \quad , \tag{A.6a}$$

$$C^{n+1} = \frac{t}{n+1} AC^n \ . \tag{A.6b}$$

The ORIGEN applies basically for all of nuclides not only the above equations but also another mathematical method depnding on a nature of decay series. That is, if the decay constant of nuclide B of the second series (produced from nuclide A) is extreme large, it is assumed that nuclide C is produced from A directly and B is obtained by an alternative technique. Furthermore, for the case where the decay constant of A is extreme large, a value of B in the transition matrix is replaced by A+B, and only the transitions of B→C is treated. These condensations of matrix are processed by the subroutine TERM. Therefore, the matrix exponential method is applied only to the case where the norm of the transition matrix is less than $2 \log_e 1000 \doteqdot 13.82$. Short-lived nuclides which ordinarily exist at the beginning of time interval, are dealt with by the Bateman equation.[18)]

The calculations for this case is carried out in the following manner. In the first step, the program searches for the transition matrix and pickes out all of rows which start from the short-lived precursors. Secondly, the Bateman equation is applied for these rows. These procedures terminate when all the short-lived precursors have been treated. Moreover, the Bateman equation is used when nuclides have the same two eigenvalues showing the existence of circular decay series. A solution of Bateman equation becomes as follows;

$$N_i(t) = N_i(0)e^{-d_i t} + \sum_{k=1}^{i-1} N_k(0) \prod_{n=k}^{i-1} \frac{a_{n+1,k}}{d_n} \left[\sum_{j=k}^{i-1} d_j \frac{e^{-d_j t} - e^{-d_i t}}{(d_i - d_j)} \prod_{\substack{n=k \\ n \neq j}}^{i-1} \frac{d_n}{(d_n - d_j)} \right], \tag{A.7}$$

where a_{ij} is the transition matrix and $d_i = -a_{i,i}$. In Eq. (A.7), the first term of right hand side is negligibly small so that only the second term on the right hand side is calculated. When $d_i t$ has a small value, a computation error will be large. However, in this case, the matrix exponential method is applied instead of the Bateman equation. Therefore, the matrix exponential method and the Bateman equation are placed in mutual compensation. In the case of having the same two decay constants ($d_i = d_j$), the summation of the second term on the right hand side in Eq. (A.7) is described as below:

$$\sum_{j=k}^{i-1} d_j t e^{-d_j t} \prod_{\substack{n=k \\ n\neq j}}^{i-1} \frac{d_n}{d_n - d_j} \quad . \tag{A.8}$$

Equation (A.8) is applied when two nuclides in one chain have the same orthogonal elements or when the circular chain exists such that the precursor of the interest elements is the same.

If a short-lived nuclide has a long-lived precursor, the following method is employed. Namely, it is assumed that a short-lived daughter nuclide is in the secular equilibrium until the end of any time interval. The concentration of the parent nuclide is calculated by the subroutine TERM and the daughter is calculated by the subroutine EQUIL by setting Eq. (A.2) equal to zero. That is,

$$\dot{X} = 0 = AX \quad . \tag{A.9}$$

Equation (A.9) is solved by the Gauss-Seidel method:

$$X_i^{k+1} = -(a_{ii})^{-1} \sum_{\substack{j=1 \\ j\neq i}}^{N} a_{ij} X_j^{k} \quad . \tag{A.10}$$

Actually, Eq. (A.10) converges rapidly because of no existence of the circular chain for these short-lived nuclides.

An application of the matrix exponential method for inhomogeneous systems is described below. This situation will occure in such cases as adding or removing fuels continuously. The matrix equation is written as follows;

$$\frac{dX}{dt} = AX + B \quad . \tag{A.11}$$

A solution of Eq. (A.11) is

$$X = [\exp(At) - I]A^{-1}B \quad . \tag{A.12}$$

Using matrix exponential function, Eq. (A.12) is described as

$$\begin{aligned} X &= [I + \frac{At}{2} + \frac{(At)^2}{3!} + \ldots.]Bt \\ &= (\sum_{m=0}^{\infty} \frac{(At)^m}{(m+1)!})Bt \quad . \end{aligned} \tag{A.13}$$

It is assumed that X is also expanded as

$$X = \sum_{n=1}^{\infty} D^n \quad . \tag{A.14}$$

Using Eqs. (A.13) and (A.14), the following equation is derived.

$$D^{n+1} = \frac{t}{n+1} AD^n \quad . \tag{A.15}$$

The short-lived nuclides are treated in the same way as mentioned in the treatment of Eq. (A.9), that is,

$$\dot{X} = 0 = AX + B \quad . \tag{A.16}$$

Equation (A.16) is solved also by the Gauss-Seidel method.

The variations of the neutron flux and the specific power during irradiation are calculated as follows in ORIGEN, by assuming that the fuel composition and the specific power are known at the start of the calculation, the neutron flux and specific power is connected by

$$P = 3.20 \times 10^{-17} \Sigma\phi V, \tag{A.17}$$

where P is the specific power in (MW), Σ is the macroscopic cross section, ϕ is the neutron flux, and V is the volume of the system. It is assumed that emitted energy per fission is 200 MeV and the time dependent neutron flux is approximated by Taylor expansion:

$$\phi(t) = 3.125\times10^{16} PV^{-1}\left[\frac{1}{\Sigma(0)} - t\,\frac{\dot{\Sigma}(0)}{(\Sigma(0))^2} + \frac{t^2}{2}\left(\frac{2[\dot{\Sigma}(0)]^2-\ddot{\Sigma}(0)\Sigma(0)}{(\Sigma(0))^3} + \ldots\right)\right]. \tag{A.18}$$

or

$$\phi(t) = \phi(0)\left[1-t\,\frac{\dot{\Sigma}(0)}{\Sigma(0)} + \frac{t^2}{2}\left(\frac{2\dot{\Sigma}(0)^2-\ddot{\Sigma}\Sigma(0)}{\Sigma(0)^2}\right) + \ldots\ldots\right]. \tag{A.19}$$

The averaged neutron flux is given by integrating Eq. (A.19) over the interval and dividing by t.

$$\bar{\phi} = \phi(0)\left[1 - \frac{t}{2}\,\frac{\dot{\Sigma}(0)}{\Sigma(0)} + \frac{t^2}{6}\left(\frac{2\dot{\Sigma}(0)^2-\ddot{\Sigma}(0)\Sigma(0)}{\Sigma(0)^2}\right) + \ldots\ldots\right], \tag{A.20}$$

where $\dot{\Sigma}$ and $\ddot{\Sigma}$ are the first and second time derivatives of Σ, respectively,

and these values can be obtained by the following two equations:

$$\dot{X}(0) = AX(0) \ , \tag{A.21a}$$

$$\ddot{X}(0) = A^2X(0) \ . \tag{A.21b}$$

The averaged power is now obtained by

$$P = 3.20\times10^{-17}\bar{\phi}V\Sigma(0)[1 + \frac{t}{2}\dot{\Sigma}(0) + \frac{t^2}{6}\ddot{\Sigma}(0) + ...]. \tag{A.22}$$

Appendix B Description of JOB Control MACRO

B-1. JOB Control MACRO

A user of ORIGEN-JR program must prepare the following JOB control MACRO for the available computer FACOM 230/75, JAERI. The section B-2 shows the assignment for the input/output files.

```
$NO
$GJOB
$HLIEDRUN RFNAME=J9001.RORIGENA
$DISKTO F01,J9001.ELIESDAT
$DISKTO F02,J0694.STOPPER
$DISKTO F10.001,J0694.ORIL 1
$DISKTO F10.002,J0694.ORIL 2
$DISKTO F10.003,J0694.ORIL 3
$DISKTO F10.004,J0694.ORIL 4
$DISKTO F10.005,J0694.ORIL 5
$DISKTO F10.006,J0694.ORIL 6
$DISK   F15
$DISK   F20
$DISKTN F21,J9001.NCDATA
$DISK   F30
$DATA
```

D A T A

```
$JEND
```

B-2. File assignment

The ORIGEN-JR requires the input/output files shown in the Table B.1 during the execution.

Table B.1 Input/Output files used in ORIGEN-JR

Logical unit number	Parameter	Comment
F01	NOPT = 1	input file for (α,n) differential cross section library
F02	NOPT = 1	input file for stopping power library
F10		input file for original library data
F15	NOPT = 1	scratch file
F20		scratch file
F21	NOPT = 1 and ID1 = 1	output file for nuclide concentrations by each time interval
F30	NGO = 10	scratch file

Appendix C Detailed Description of ORIGEN-JR Subroutines

The name of the various subroutines, their major functions, and the important variable names in each routine are described below in the order that they are employed in the code.

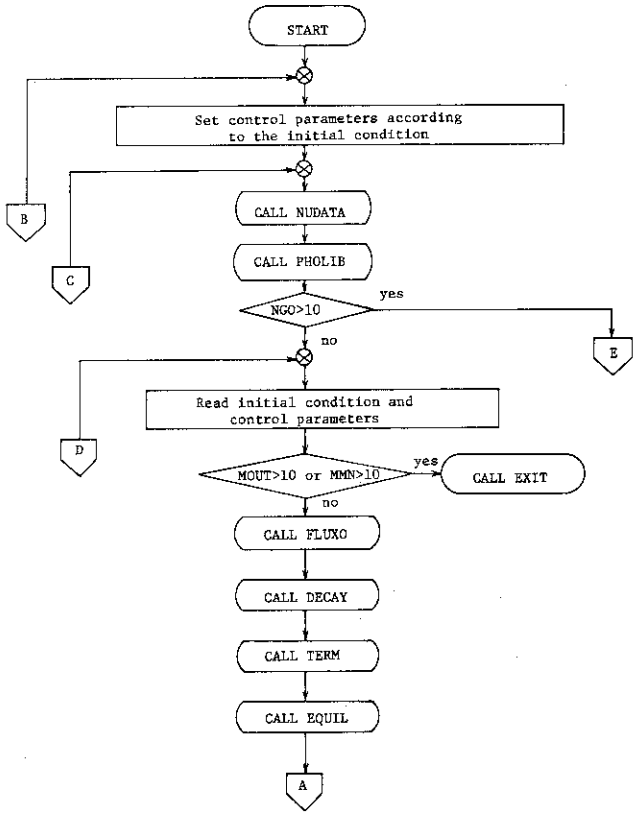
C-1, FTMAIN

This is the program that supervises the execution of tasks of other routines. The code solves a set of first order, linear, ordinary differential equations:

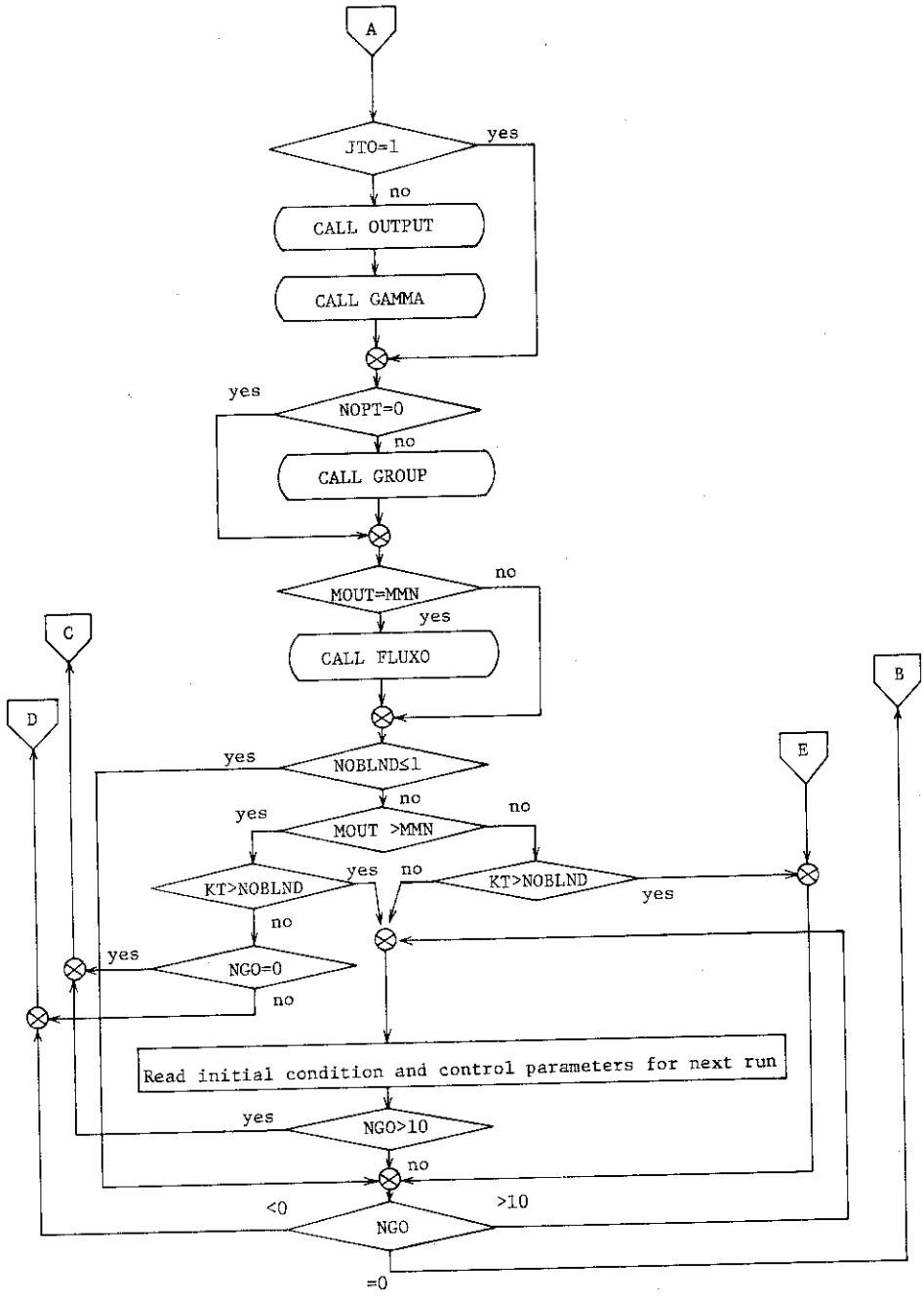
$$\dot{X} = AX + B, \text{ given } X(0),$$

where X(0) is a set of initial concentrations, X(t) is the time-dependent solution to be obtained, A is a matrix of first-order rate coefficients, and B is a forcing vector. In the code, the variables A and B have the name A and B, respectively, the variable X(0) has the name XZERO, and the solution has the name XNEW. These variables are stored in labeled common blocks /MATRIX/ and /EQ/.

FTMAIN



FTMAIN (Cont.)

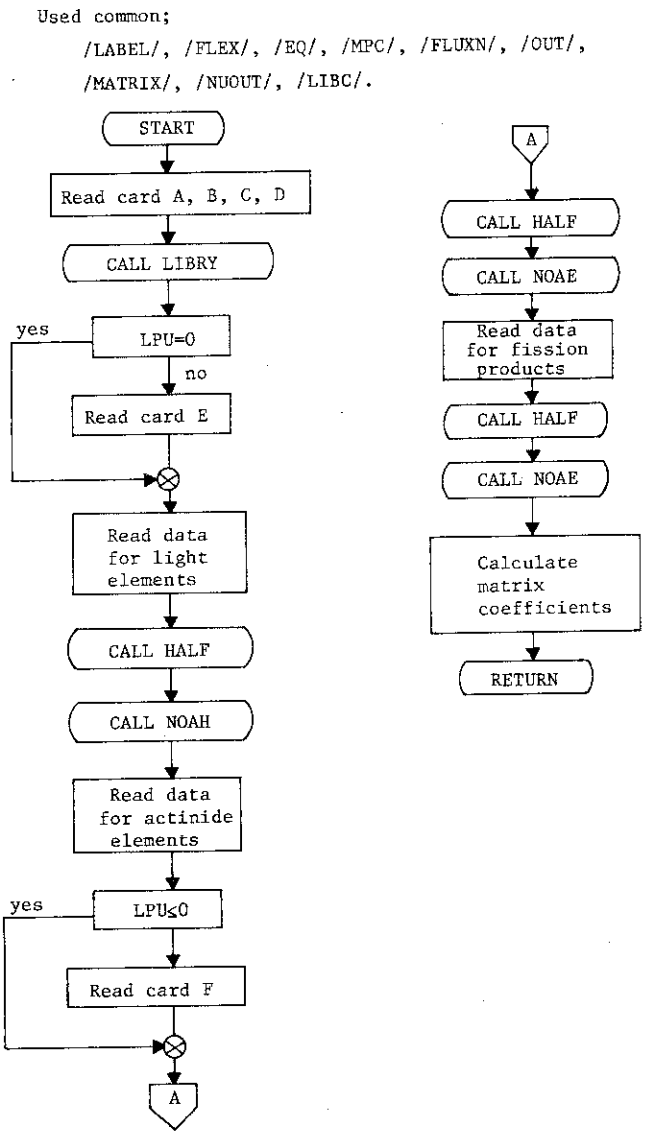

A
JTO=1
yes
no
CALL OUTPUT
CALL GAMMA
yes
NOPT=0
no
CALL GROUP
no
MOUT=MMN
yes
CALL FLUXO
C
B
D
E
yes
NOBLND≤1
no
yes
MOUT >MMN
no
KT>NOBLND
yes
no
KT>NOBLND
yes
no
yes
NGO=0
no
Read initial condition and control parameters for next run
yes
NGO>10
no
<0
>10
NGO
=0

C-2, NUDATA

The subroutine NUDATA processes the nuclear data from the library tape and constructs a part of the transition matrix A. The subroutine reads the data from the library tape, updates one-group cross sections, and prints out the library of data to be used in the calculations.

The nonzero, off-diagonal terms of the matrix A are stored in the variable A. Three integer vectors, LOC, NONO and KD, are also constructed to be used to locate the matrix elements. These variables are stored in a labeled common block /MATRIX/.

Subroutine NUDATA



C-3, LIBRY

This routine processes the one-group cross section from card or file, and reconstructs part a of the transition matrix.

C-4, HALF

This subroutine computes the radioactive decay constant in units of sec^{-1}, when the half-life of the radionuclide is given in units designated by the variable IU.

C-5, NOAH

This subroutine constructs a three-word alphameric symbol for an isotope from its six-digit identifying number. The three words consist of the symbol for the chemical element, the atomic weight, and either a blank or an "M" to designate a ground or metastable state, respectively. These symbols are used only when printing output tables.

C-6, BLOCK DATA

BLOCK DATA is used to initialize variables in a labeled common block /LABEL/. These variables consist of an array of chemical symbols, ELE, and a variable to designate the isomeric state of a nuclide, STA. These arrays are used in conjunction with the subroutine NOAH.

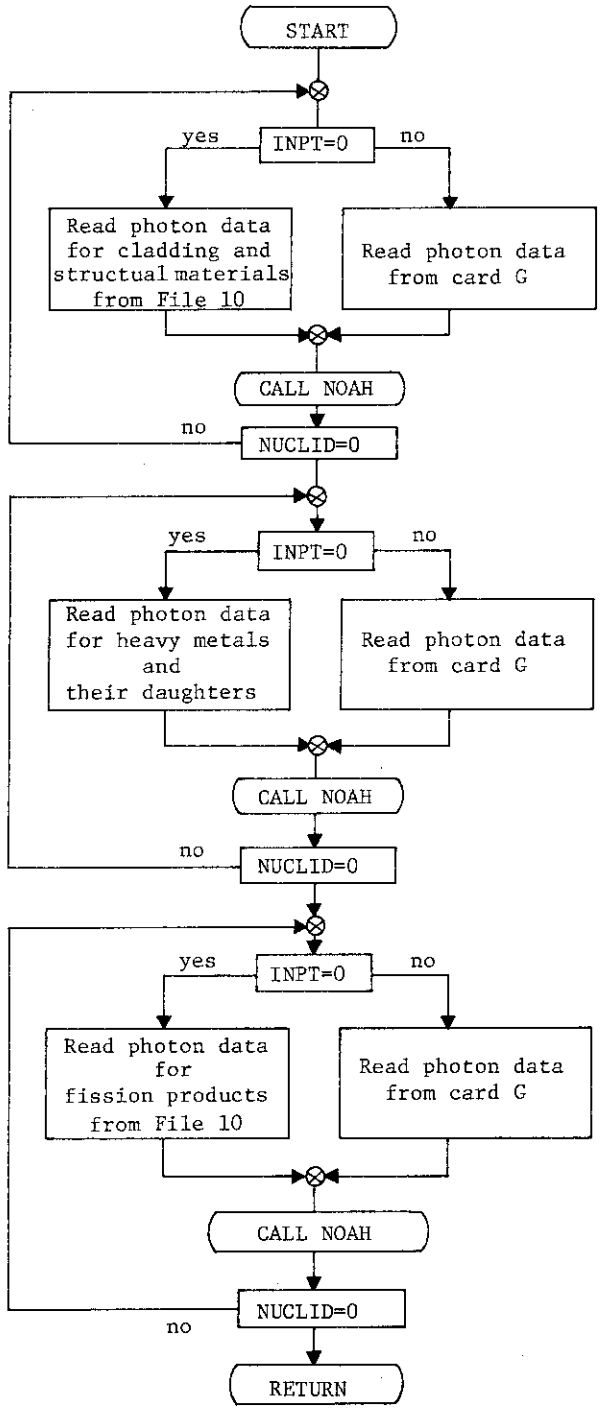
C-7, PHOLIB

The PHOLIB reads the multigroup photon production data from the nuclear library tape and stores the information in the arrays GAMGRP and ACTGRP. The array GAMGRP contains 12-energy-group photon production data for isotopes of cladding and structural materials and of fission products, while the array ACTGRP contains 18-energy-group data for isotopes of actinide elements and their radioactive decay danghters.

This subroutine also prints a table containing the data in the library.

Subroutine PHOLIB

Used common; /FLUXN/, /FLEX/, /PHOTON/, /OUT/, /NUOUT/.



C-8, FLUXO

This subroutine uses a Taylor series expansion about the computational time interval to estimate: (1) the average flux during the interval, when the reactor power is given; or (2) the average power generated by the fuel during the interval, when the neutron flux is given. Once the flux has been obtained, it is multiplied by the cross sections to generate first-order rate constants for production and destruction of nuclides by neutron-induced reactions.

The subroutine also constructs the diagonal matrix element for each isotope from the sum of the disintegration constant, the product of the spectrum-averaged total absorption cross section and the flux, and the rate coefficient for other removal processes that are propotional to the instantaneous concentration (e.g., leakage or first-order chemical reaction). The diagonal matrix elements are stored in the array D in a labeled common block /EQ/.

C-9, DECAY

This subroutine solves the Bateman equations for nuclides that appear at the beginning of decay chains and have half-lives that are short compared to the time interval for the calculation (time interval greater than 10 half-lives). The concentrations of the short-lived nuclides at the end of the interval are contained in the array XNEW, and the concentrations of any long-lived or stable daughters at the start of the interval are augmented by the amount that the short-lived precursor has decayed. The variable XTEMP is used to contain the adjusted initial concentrations of the long-lived and stable materials. The variables are stored in a labeled common block /EQ/.

C-10,TERM

The subroutine TERM has two principal functions. It constructs first a reduced coefficient matrix related to transitions between only long-lived or stable nuclides. By way of explanation, if a chain A → B → C exists, in which isotope B is short-lived while isotopes A and C are long-lived, a matrix element is created for the event A → C directly and is entered into the array AP. The array AP is a local variable that is used in the subroutine TERM. The second function of TERM is to solve the reduced system of equations that results from excluding the short-lived nuclides. The

equations are solved by the matrix exponential method, using algorithm which involves the use of a recursion relation to generate the matrix exponential function. The solution for the concentrations of long-lived and stable nuclides at the end of time interval is contained in the array XNEW.

C-11,EQUIL

The subroutine EQUIL is used to place short-lived daughters in secular equilibrium with long-lived parents. The subroutine uses the Gauss-Seidel successive substitution algorithm to solve a set of linear algebraic equations. The resulting concentrations are contained in the array XNEW.

C-12,OUTPUT

As its name indicates, this subroutine produces tables of output containing the properties of irradiated materials. OUTPUT uses the array XNEW which contains the concentrations of the fuel as a function of time, and other arrays containing the radioactive decay constant, the heat per disintegration, etc. From these, it computes inventories, radioactivities, thermal powers, and other properties of interest. It prints tables of properties of individual isotopes and of chemical elements, and prepares summary tables about the most important contributions.

C-13,GAMMA

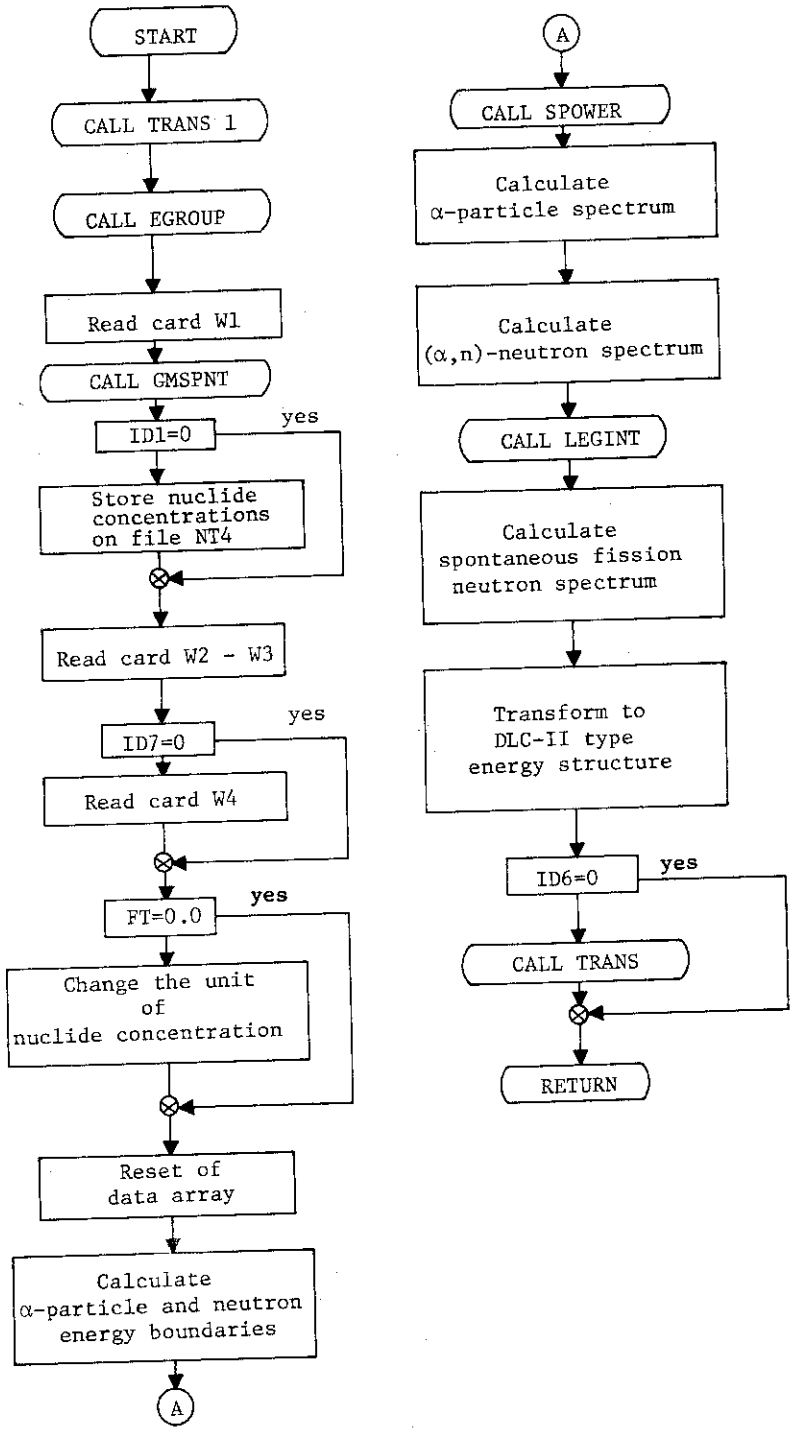
This subroutine prepares tables of penetrating radiation source in spent fuels. Using the isotopic compositions in the XNEW array, the photon release data in a labeled common block / PHOTON /, and the neutron production data in a labeled common block / OUT /, GAMMA compiles tables of multigroup photon release rates and neutron production rates as a function of time.

C-14,GROUP

This subroutine calculates the spectrum of neutrons produced by (α,n) reactions and spontaneous fissions. The original ORIGEN computes only the source intensity of neutrons, while this subroutine computes the detailed information of neutron source energy spectrum. This routine also controls the subroutine GMSPNT and TRANS. Calculated quantities are stored in a labeled common /MATRIQ/.

Subroutine GROUP

Used common; /DATAOK/, /MATRIQ/, /ALPHA/, /EQ/, /FLEX/, /FLUXN/, /OUT/, /RESULT/, /LABEL/.

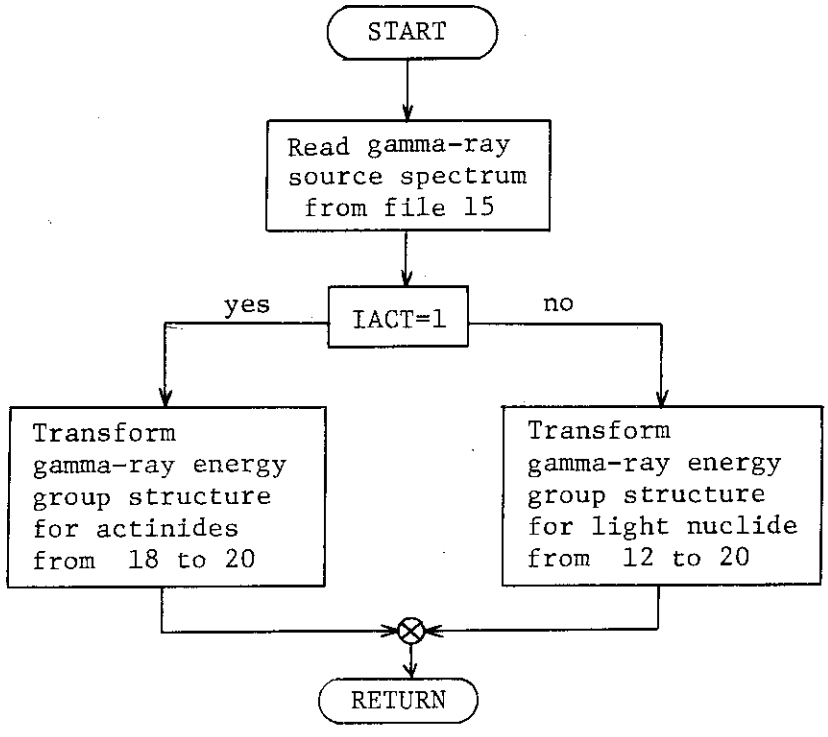


C-15, GMSPNT

This subroutine calculates γ-ray source spectrum in 20-group structure (EURLIB type) from the ORIGEN original data.

Subroutine GMSPNT

Used common; /RESULT/



C-16, TRANS1

This routine has the same role as HALF. It is used only by the subroutine GROUP.

C-17,EGROUP

This subroutine produces the neutron energy group boundary of DLC-II type for shielding calculations.

C-18,SPOWER

The SPOWER calculates interpolation value of stopping power. The interpolation is performed linearly with respect to lethargy.

C-19,LEGINT

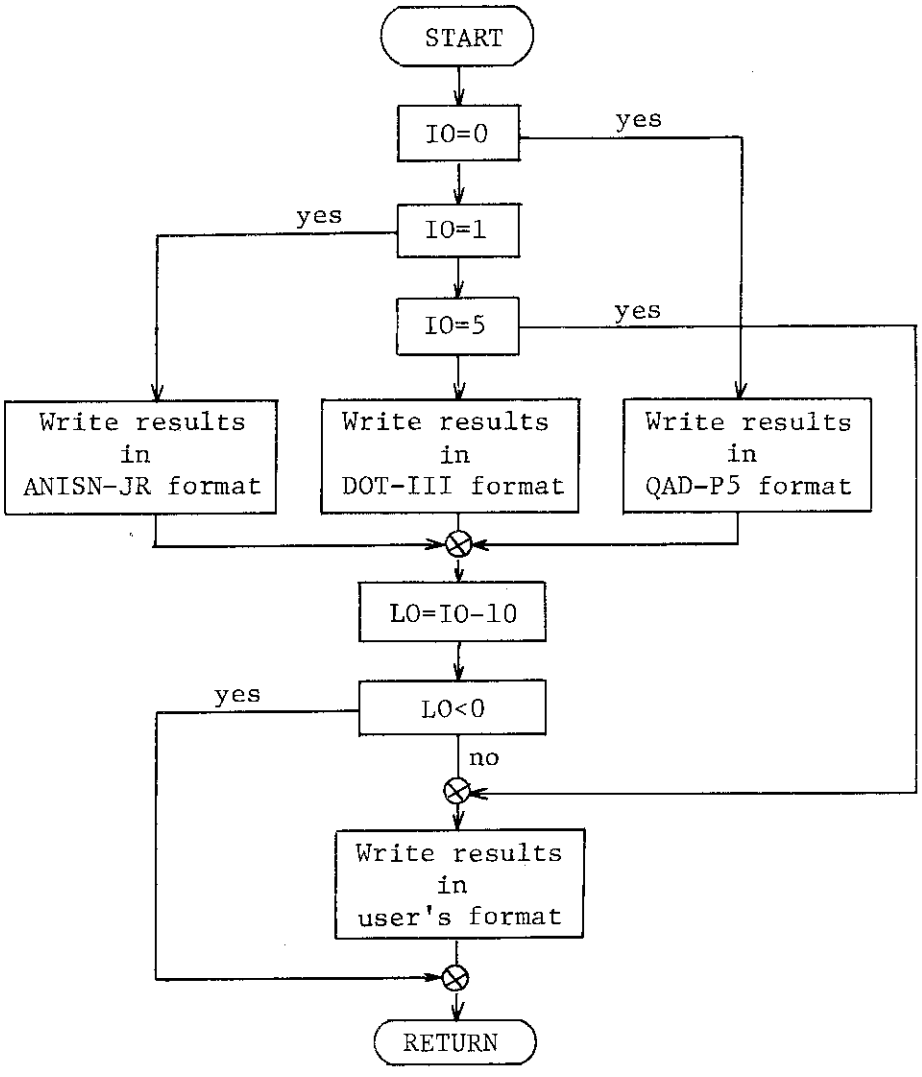
This subroutine calculates the integral values of Legendre functions P_0 to P_ℓ, if it is assigned L. These results are entered into one dimensional matrix FX.

C-20,TRANS

This subroutine produces input source data of neutrons and gamma rays for shielding calculations by the codes, QAD-P5, ANISN-JR and DOT-III, from the results stored in a labeled common /RESULT/ calculated by the subroutines GMSPNT and GROUP.

Subroutine TRANS

Used common; /RESULT/



C-21, BLOCK DATA MODFY

BLOCK DATA MODFY is used to initialize the variables in a labeled common block / DATAOK /. These variables are used only in the subroutine GROUP.

Table C.1 Definitions and storage locations of important variables.

A	/ MATRIX /	transition matrix
ABUND	/ OUT /	isotopic abundances of cladding and structural materials, (at. %)
ALPHAN	/ OUT /	number of neutrons produced per alpha disintegration by heavy metal isotopes
ASPRM (I, J)	/ MATRIQ /	calculated α-particle energy spectrum by actinide nuclides. I and J are identification of actinide nuclides and α-particle energy, respectively.
ANSPM	/ MATRIQ /	α-particle energy spectrum summed over actinide nuclides
ABD	/ DATAOK /	fraction of emitted α-particle energy
ADC	/ MATRIQ /	α-decay constant of the actinide (1/sec)
AMPC	/ MPC /	radioactivity concentration guide for continuous inhalation in unrestricted areas ($\mu Ci/cm^3$)
B	/ EQ /	forcing vector
D	/ EQ /	diagonal matrix elements
DIS	/ FLUXN /	radioactive decay constant (1/sec)
DLIB	/ DATAOK /	α-decay constant used only in the subroutine GROUP
DLIB 1	/ DATAOK /	spontaneous fission decay constant used only in the subroutine GROUP
DAE	/ MATRIQ /	concentration of actinides for calculation of (α,n) neutron source
DLE	/ MATRIQ /	concentration of light nuclides for calculation of (α,n) neutron source
DME	/ MATRIQ /	concentration of structural nuclides for calculation of (α,n) neutron source
FG	/ OUT /	fraction of radioactive decay energy resulting from photons with energies above 200 keV
FISS	/ FLUXN /	spectrum averaged fission cross section (barns)
NUCL	/ OUT /	six-digit integer constant used to identify isotopes
MUCL	/ DATAOK /	ibid.
Q	/ OUT /	radioactive decay energy released as recoverable heat (MeV / disintegration)
SPONF	/ OUT /	spontaneous fission rate for heavy metal isotopes (fissions / sec-atom)

TOCAP	/ FLUXN /	total spectrum-averaged neutron absorption cross section (barns)
WMPC	/ MPC /	radioactivity concentration guide for continuous ingestion in unrestricted areas ($\mu Ci/cm^3$)
EAE (I, J)	/ DATAOK /	emitted alpha-particle energy in L.M.S.(eV) I and J indicate number of emitted energy and actinide nuclides, respectively
PROB	/ DATAOK /	frequency of α-decay mode
PROB 1	/ DATAOK /	frequency of neutron-decay mode
NOAE	/ MATRIQ /	identification number of actinide nuclides
NOLE	/ MATRIQ /	identification number of light nuclides
NOME	/ MATRIQ /	identification number of structural nuclides
SMS (I,J,K)	/ MATRIQ /	calculated (α,n) neutron spectrum by each light nuclide and energy level.
SUM (I,J)	/ MATRIQ /	calculated (α,n) neutron spectrum summed over each energy level.
SUMM (I)	/ MATRIQ /	calculated (α,n) neutron spectrum summed over each light nuclides.
EGN	/ MATRIQ /	neutron energy boundaries (eV)
UGN	/ MATRIQ /	neutron lethargy boundaries
EGA	/ ALPHA /	α-particle energy boundaries (eV)
UGA	/ ALPHA /	α-particle lethargy boundaries
SP	/ ALPHA /	stopping power ($eV \cdot cm^2/g$)
SYBL	/ MATRIX /	spin-parity of residual nuclide
SFSPM	/ MATRIX /	spontaneous fission neutron spectrum
SPW	/ MATRIX /	stopping power of calculational material (eV/cm)
BL (I,J,K)		Legendre coefficients of (α,n) cross section. I, J and K are α-particle energy, residual level, and order of the Legendre function, respectively.
SPIN1		excitation energy of the residual nuclide (eV)
FY		integral value of the Legendre coefficients
E		neutron energy boundareis of the DLC-2 type group structure.

Appendix D Description of Data Libraries added to ORIGEN-JR

An extensive library of nuclear data has been compiled and recorded on a disk file for use with the ORIGEN-JR code. In addition, the following two libraries have to be prepared for use with the ORIGEN-JR code, that is,

1) stopping power library.
2) (α,n) reaction data library.

D-1. Stopping power library

This library contains energy dependent stopping powers for 58 materials. The library is read as follows;

READ(NT2) MAT, ROW, (SP(I), I=1, 14),

where

MAT ; identification number of isotope (this form is the same as for NUCL),

ROW ; density of the nuclide (g/cm^3),

SP(I); energy depndent stopping power. ($eV \cdot cm^2/g$)

Energy points are shown in Table D.1.

Table D.1 Energy points of stopping power library

I	Energy (MeV)	Lethargy
1	0.6	2.81341
2	0.7	2.65926
3	0.8	2.52573
4	1.0	2.30259
5	1.5	1.89712
6	2.0	1.60944
7	3.0	1.20397
8	4.0	0.91629
9	5.0	0.69315
10	6.0	0.51083
11	7.0	0.35668
12	8.0	0.22314
13	10.0	0.0
14	15.0	-0.40547

D-2. (α,n) reaction data library

This library consists of (α,n)-differential cross sections, Q-values and energy levels for target nuclides, ^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O and ^{19}F. The (α,n) differential cross sections are tubulated in the form of Legendre coefficients. The Q-values and energy levels are given in units of eV. The library is read as follows;

```
      READ(NT1)   NMAT, NMAX, (MATNO(I), I=1, NMAX)
      DO  1   I=1, NMAX
      READ(NT1)   MAT, ILEV, IEA, Q, (EPL(J), J=1, ILEV)
      DO  1   K=1, ILEV
1     READ(NT1)   LEVEL(K), SPIN(K), ((BL(J,K,L), L=1, 11), J=1, IEA)
```

where

NMAT ; identification number of (α,n) library,
NMAX ; number of light nuclides contained in this library,
MATNO; identification number of light nuclide,
MAT ; identification number of light nuclide in this data section,
ILEV ; number of energy levels for the residual nuclide (normally 5),
IEA ; number of α-particle energy points (normally 100),
Q ; Q-value (eV),
EPL ; residual nuclide energy levels (eV),
LEVEL; identification number of energy level in this data section,
SPIN ; spin of the residual nuclide (its sign stands for the parity),
BL ; (α,n)-differential cross sections in the form of the Legendre coefficient.

Appendix E User's Manual for Utility Codes

E-1. Functions and Input Instructions of Utility Codes

E-1.1. ELIESE5

Differential cross sections of (α,n) reactions are prepared by the code by using a same procedure based on the statistical model as in the ELIESE-3[19] code. The library of the (α,n) reaction cross sections generated by the code are used for estimating of neutron yields and energy spectra due to (α,n) reactions.

E-1.1a. Input Instruction of ELIESE5

CARD 1. Control card. Format (I10, 6I5, E12.5)

MATNO ; identification number of light nuclide,
NT ; logical unit number for a output tape of the Legendre coefficient table,
IIIB ; the first number of α-particle energy (set to 1),
IIIE ; the last number of α-particle energy (set to 100),
INTVL ; mesh spacing of α-particle energy (set to 1),
IPR1 ; number of residual nuclide energy levels,
IPR2 ; number of angular mesh points,
QVALUE ; Q-value of (α,n) reaction (eV).

CARD 2. ELIESE3 original input

This part of input data is same as that of ELIESE3. Detailed description is noted in the reference 19.

E-1.2. EDITLIB

This code edits data files produced by ELIESE5 and updates the (α,n) data library. The functions of this code are as follows;

1) put together the cross section files of many nuclides into one file.
2) edit a new cross section file of the form 1 mentioned below.
3) update the cross section values for any energy groups and excitation levels for any nuclides by data card or tape of the form 1 or 2 mentioned below.

The forms of the cross section files are as follows (definitions of variables are described in Appendix D);

Form 1

```
MAT , Q, ILEV, (EPL(I),I=1,ILEV)
DO 100  J=1,IEA
DO 100  K=1,ILEV
100 WRITE(ID) LEVEL(K),SPIN(K),(BL(J,K,L),L=1,11)
```

Form 2

```
WRITE(ID) NMAT,NMAX,(MATNO(I),I=1,NMAX)
DO 100  I=1,NMAX
WRITE(ID) MAT,ILEV,IEA,Q,(EPL(J),J=1,ILEV)
DO 100  K=1,ILEV
100 WRITE(ID) LEVEL(K),SPIN(K),((BL(J,K.L),L=1,11),J=1,IEA)
```

E-1.2a. Input Instruction of EDITLIB

CARD 1. Control card. Format (4I10)

KF ; selection of operating functions,
0 - edit or replace,
1 - update by data card,
2 - update by data tape,
3 - renormalization only.

ID1 ; ligical unit number of an old data library to be edited or updated (the tape written by form 2 can only be assigned).

IM ; number of tape or card to edit or update (if KF=1,IM means number of cards).

NNMAT; new identification number of the (α,n) data library for updating or replacing.

The following input cards, 2-1 to 2-5, must be repeated IM times when KF=0 and IM≠0. If materials with same identification number exist in the old and the new libraries, old values are replaced by new one.

CARD 2-1. Format (4I10)

ID2 ; logical unit number of the (α,n) data file.

MAT ; identification number of a material in the library.

IRL ; number of the residual nuclide excitation levels.

JFN ; selection of renormalization factors,
0: no change,
1: each level and energy,
2: each level,
3: all of them.

CARD 2-2. Format (5F12.8,20X)

SPIE(I),I=1,IRL ; energy of residual nuclide excitation level (MeV)

CARD 2-3. (JFN=1) Format (5F12.8,20X)

(FN(I,L),L=1,IRL),I=1,100) ; values of renormalizations.

CARD 2-4. (JFN=2) Format (5F12.8,20X)

(FN(L),L=1,IRL) ; ibid.

CARD 2-5 (JFN=3) Format (5F12.8,20X)

FN ; ibid.

The following input cards, 3-1 to 3-2, must be repeated IM times when KF=1 and IM≠0.

CARD 3-1. Format (4I10)

MAT ; identification number of the material to be updated.

ILV ; identification number of the excitation level to be updated.

IEU ; identification number of energy to be updated.

CARD 3-2. Format (6E12.4,8X)

(BL(J),J=1,11) ; Legendre coefficients to be updated.

The following input cards, 4-1 to 4-2, must be repeated IM times when KF=2 and IM≠0.

CARD 4-1. Format (4I10)

ID2 ; logical unit number of the (α,n) data library to be updated.

MAT ; identification number of the material to be updated.

JFT ; form of the library,
1 - form 1,
2 - form 2.

IRL ; number of excitation levels.

ILV ; level number to be updated (if ILV=0, all levels are updated).

CARD 4-2. (JFT=1) Format (5F12.8,20X)
(SPIE(I),I=1,IRL) ; energy of residual nuclide excitation level (MeV).

The following input cards, 5-1 to 5-4, must be repeated IM times when KF=3 and IM≠0.

CARD 5-1. Format (4I10)

MAT ; identification number of the material.

JFN ; selection of the renormalization,
0 - no change,
1 - each level and energy,
2 - each level,
3 - all of them.

CARD 5-2. (JFN=1) Format (5F12.8,20X)
(FN(I,L),L=1,5),I=1,100) ; values of the renormalizations.

CARD 5-3. (JFN=2)
(FN(L),L=1,5) ; ibid.

CARD 5-4. (JFN=3)
FN ; ibid.

E-1.2b. JOB Control MACRO of EDITLIB

The JOB control MACRO of EDITLIB for FACOM 230/75 is described below. This MACRO is used in a case of the file edition and the format conversion from the (α,n) data files on the logical units, F10 ∿ F17, written by the

form 1 to the logical unit, F02, written by the form 2. The logical units, F10 ∿ F17, are assigned in the data cards, so that these can be changed by user.

```
$NO
$GJOB
$HLIEDRUN  RFNAME=J9001.REDITLIB
$DISKTO  F10,J9001.NBLBE9
$DISKTO  F11,J9001.NBLB10
$DISKTO  F12,J9001.NBLB11
$DISKTO  F13,J9001.MBLC13
$DISKTO  F14,J9001.NBLN14
$DISKTO  F15,J9001.NBLO17
$DISKTO  F16,J9001.NBLO18
$DISKTO  F17,J9001.NBLF19
$DISKTN  F02,J9001.EDITLIB
$DISK    F20
$DISK    F21
$DISK    F22
$DATA
```

DATA

```
$JEND
```

E-1.2c. File assignment

EDITLIB requires the input/output files as shown in the Table E.1.

Table E.1 File assignment of EDITLIB

Logical unit number	Parameter	Comments
F02		output file for new (α,n) data library.
F20		scratch file.
F21		scratch file.
F22		scratch file.
F01	ID1=1	input file for the old (α,n) data library it can be changed by user.
F10	ID2=10	input file for the (α,n) data library to be edit or replace. it can be changed by user.

E-1.3. LISTLIB

This code is used for listing the (α,n) data and the stopping power values on the library.

E-1.3a. Input Instruction of LISTLIB

CARD 1. Title card. Format (10A4)

CARD 2. Control card. Format (2(9X,A1),A1,9X,I10)

AS ; selection of library,
A - (α,n) data library of form 1,
B - (α,n) data library of form 2,
C - Stopping power table.

BS ; selection of print form (AS≠C),
A - print cross section by angle,
L - print cross section by the form of the Legendre expansion.

CS ; additional option (AS≠C and BS=A),
blank - print cross section only 10 angles,

D - print detailed information.

MAT ; material number of light nuclide, this option is only used when AS≠C.

E-1.3b. JOB Control MACRO of LISTLIB

The JOB control MACRO of LISTLIB for FACOM 230/75, JAERI is as follows;

```
$NO
$GJOB
$HLIEDRUN  RFNAME=J9001.RLISTLIB
$DISKTO  F01, J9001.EDITLIB
$DATA
```

DATA

```
$JEND
```

Note; the logical unit number F01 must be assigned as input file.

E-1.4. ALPHAN

This code is prepared for calculating the detailed neutron source spectrum at the each cooling time step by using the nuclide concentration data tape produced by ORIGEN-JR. Also calculation is available for arbitrary values of nuclide concentration given by data cards.

E-1.4a. Input Instruction of ALPHAN

CARD 1. Control card. Format (7I5,2E12.5)

ID1 ; 1 - read values of nuclide concentration from a tape on logical unit 21,
0 - read values of nuclide concentration from cards.

ID2 ; 1 - print α-particle energy spectrum,
0 - no effect.

ID3 ; 1 - print detailed information of neutron source spectrum,
0 - no effect.

ID4 ; 1 - print (α,n) neutron source spectrum by each light nuclide,
0 - no effect.

ID5 ; 1 - calculate spontaneous fission neutron spectrum,
0 - no effect.

ID6 ; 1 - punch source data for the shielding calculation codes,
0 - no effect.

ID7 ; 1 - read data of structural nuclide,
0 - no effect.

FT ; conversion factor of units for values of nuclide concentration (if FT=0.0 is entered, the unit of nuclide concentration is gram-atom).

V ; volume of the source region for the shileding calculation (cm^3).

CARD 2. Assignments of actinides. Format (8I10)

NAE ; number of actinide nuclides for the calculation,
(NOAE(I),I=1,NAE); nuclide identification number.

CARD 3. Assignments of light nuclides. Format (8I10)

NLE ; number of light nuclides for the calculation,
(NOLE(I),I=1,NLE); nuclide identification number.

CARD 4. Assignments of structural nuclides. Format (8I10) (ID7≠0)

NME ; number of structural nuclides for the calculation,
(NOME(I),I=1,NME); nuclide identification number.

CARD 5. Control for punched card format. Format (20I4) (ID6≠0)

IO ; selection of shielding calculation code,
0 - QAD-P5,
1 - ANISN,
2 - DOT-III,
5 - output for user's format,
10 - QAD-P5 and user's format,
11 - ANISN and user's format,
12 - DOT-III and user's format.

IM ; number of total mesh intervals (IO=1 or 11).

IIM ; first interval number of source region (IO=1 or 11).

IIS ; number of mesh intervals of source region (IO=1 or 11).

IEQ ; number of few group.

Detailed definition of these parameters is same as the card I of ORIGEN-JR.

CARD 6. Few group parameters. Format (20I4) (IEQ>0)

(IQB(I),I=1,120); few group number for each multigroup.

Note; $1 \leq I \leq 100$ are corresponded to neutron groups and $101 \leq I \leq 120$ are of no use in the code. Detailed description is same as the card J of ORIGEN-JR.

CARD 7. Values of concentration. Format (8E10.3) (ID1=0)

(DAE(I),I=1,NAE); values of actinide nuclides.

CARD 8. Values of concentration. Format (8E10.3) (ID1=0)

(DLE(I),I=1,NLE); values of light nuclides.

CARD 9. Values of concentration. Format (8E10.3) (ID1=0 and ID7=1)

(DME(I),I=1,NME); values of structural nuclides.

Note; values of nuclide concentration are given in units of gram-atom when FT=0.0.

E-1.4b. JOB Control MACRO of ALPHAN

The JOB control MACRO of ALPHAN for FACOM 230/75, JAERI is as follows;

```
$NO
$GJOB
$HLIEDRUN    RFNAME=J9001.RALPHAN
$DISKTO    F01,J9001.ELIESDAT
$DISKTO    F02,J0694.STOPPER
$DISKTO    F21,J9001.ORIGOUT
$DATA
          DATA
$JEND
```

E-1.4c. File assignment

ALPHAN requires the input/output files as shown in the Table E.2.

Table E.2 File assignment of ALPHAN

Logical unit number	Parameter	Comments
F01		(α,n) data library.
F02		stopping power library.
F21	ID1=1	nuclide concentrations calculated by ORIGEN-JR

The schematic diagram of these utility codes is shown in Fig. E.1.

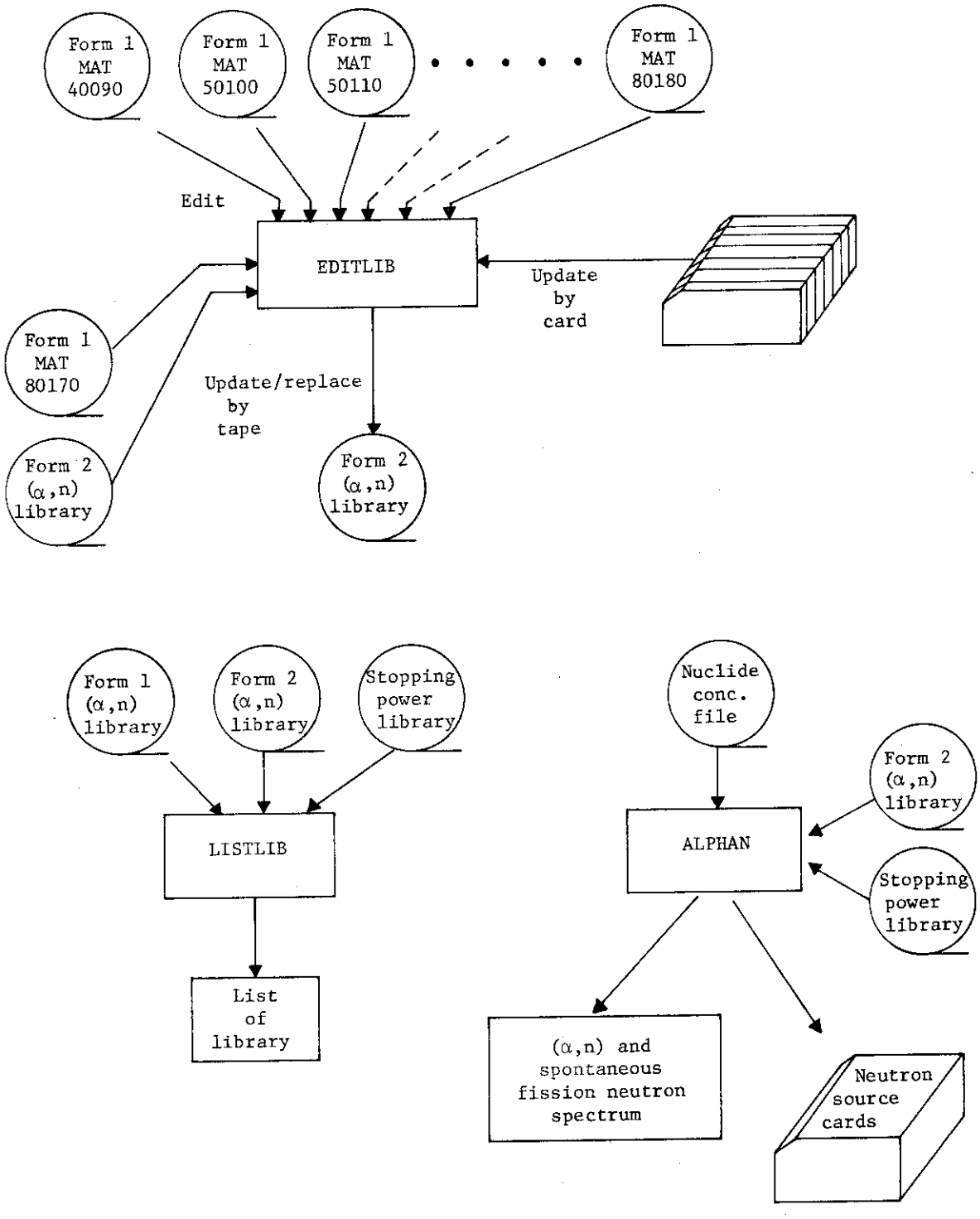


Fig.E.1 Schematic diagram of utility code

a list of errata

page	line	erratum	correct
6	15	method.	method.[4)]
10	26	IEQ=20	IEQ=24
10	29	20.	20.....
11	6	card 23 ··· group 20	card 26 ··· group 24
11	7	card 24	card 27
12	caption of Fig.3	+Number of ··· 20 ···	+Number of ··· 24 ···
36		NOPT=1	NOPT≠0
42	7	neutron-	neutron