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MACK-IV, A New Version of MACK:

A Program to Calculate Nuclear Response Functions from Data in ENDF/B Format

by

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Computer Code Abstract

MACK-IV

1. Program Identification

MACK-IV[1] an expanded version of MACK:[2] A program to calculate Nuclear Response Functions from basic nuclear data in ENDF/B format.[3]

2. Description of Physical Problem Solved

MACK-IV calculates nuclear response functions important to the neutronics analysis of nuclear and fusion systems. A central part of the code deals with the calculation of the nuclear response function for nuclear heating more commonly known as the kerma factor.[4] Pointwise and multigroup neutron kerma factors, individual reactions, helium, hydrogen, and tritium production response functions are calculated from any basic nuclear data library in ENDF/B format. The program processes all reactions in the energy range of 0 to 20 MeV for fissionable and nonfissionable materials. The program also calculates the gamma production cross sections and the gamma production energy matrix. A built-in computational capability permits the code to calculate the cross sections in the resolved and unresolved resonance regions from resonance parameters in ENDF/B with an option for Doppler broadening. All energy pointwise and multigroup data calculated by the code can be punched, printed and/or written on tape files. Multigroup response functions (e.g., kerma factors, reaction cross sections, gas production, atomic displacements, etc.) can be outputted in the format of "MACK-ACTIVITY-Table" suitable for direct use with current neutron (and photon) transport codes.

3. Method of Solution

The neutron kerma factor, whose calculation is a central part of MACK-IV is obtained by summing over all possible neutron reactions, the product of th reaction cross section and the energy deposited in the reaction within a negligible distance from the site of collision. The energy deposited in a reaction is the sum of the kinetic energies imparted to the recoil nucleus and charged particles emitted. This is calculated from an energy balance that accounts for mass-to-energy conversion and the energies carried away from the site of collision by neutrons and secondary gamma rays. The kinetic energy o the neutrons is calculated from the angular or the energy distributions given in ENDF/B data files. The part of the reaction energy carried away with the gamma rays is calculated by one of two methods that can be selected by the user. In the first method, the gamma energy is calculated directly from info mation in the gamma production files of ENDF/B. In the second method, the gamma energy is deduced from solving all the nuclear kinematics equations (momentum as well as energy balance) assuming that direct inforamtion on gamm production is not available. The calculation of cross sections in the resonance region follows that of the NPTXS module in the AMPX[5] system. Multigroup kerma factors and cross sections are calculated using an arbitrary weighting function. The gamma production cross sections are calculated from the gamma production files in ENDF/B. The code ensures the consistency in preserving the energy in all phases of the nuclear heating calculations.

4. Related Materials

The program is self-contained and no auxiliary programs are needed. A basic nuclear data library in ENDF/B format is required.

5. Restrictions

The main restriction is the availability of the computer core storage. The program utilizes the dynamic storage technique to save on core storage requirements.

6. Computer

IBM-370 models 195 and 158, UNIVAC-1110 (also compatible with CDC-7600 with minor modifications).

7. Running Time

The problem run time depends mainly on (a) number of resolved resonances; (b) size of the pointwise energy mesh; (c) method selected for calculating kerma factor; and (d) number of neutron and gamma energy groups. Typical CPU time is 1-3 min for nonresonance nuclides and 5-10 min for resonance nuclides on IBM-370/195 with 1000 energy points, 21 neutron groups, and 36 gamma energy groups.

8. Programming Languages

The code is written in FORTRAN IV.

9. Operating System

Normal operating systems for one FORTRAN programs.

10. Machine Requirements

The central memory storage requirements vary but are typically within 400 to 800 K bytes. The input/output and temporary files vary from 4 to 13 depending on the problem.

11. Material Available

Source program, test problems, results of executed test problems, and a program report. This package can be obtained through the Radiation Shielding Information Center at Oak Ridge National Laboratory, and the Argonne Code Center at Argonne National Laboratory.

12. Acknowledgment

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13. References

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I. INTRODUCTION

A major part of the neutronics and photonics analyses of a nuclear system involves estimating a set of nuclear response rates such as nuclear heating, gas production, and atomic displacements rates. These response rates provide an important input to the engineering design and analysis of the system. The calculation of a nuclear response requires an integration over the appropriate phase space of the product of the neutron (or gamma) flux and a nuclear response function. A primary function of the MACK computer program is to calculate important response functions from basic nuclear data in ENDF/B format.

The MACK[1] program has evolved from a strong need in the fusion field for such a capability. The high energy of the neutrons from the D-T reaction, the variety of nuclear reactions that can be induced at such high energy, and some unique features of the fusion systems made it necessary to depart from the rather simple models commonly employed in fission systems and develop new comprehensive and accurate methodology for calculating the nuclear response functions; the most complex of which is that for nuclear heating commonly known as kerma factor. The first version of MACK[1] was released in 1973. This early version has been used extensively with great success in many nuclear applications in addition to the neutronics analysis of fusion reactors.

This report describes the new version of MACK designated as MACK-IV. The new version involves expansion in the scope of the program, the addition of new important capabilities, improvement in calculational algorithms, and is intended for applications in general nuclear systems as well as the fusion reactors. The major features of MACK-IV can be summarized as follows:

(1) All reactions including fission that are significant in the energy range 0-20 MeV and are currently defined in ENDF/B format (Version IV) can be processed for all materials.

(2) The calculational algorithms for neutron kerma factors maximize the utilization of nuclear data. Two methods are included to provide the best possible accuracy with and without the availability of direct information on secondary gamma-ray production.

(3) The gamma-production cross sections can be calculated so as to ensure consistency in preserving the energy in all phases of the nuclear (neutron plus gamma) heating calculations.

(4) Cross sections can be calculated in the resolved and unresolved resonance regions from resonance parameters in file 2 of ENDF/B with a capability for Doppler broadening.

(5) A single response function is calculated for each type of gas production (helium, hydrogen, and tritium) from individual neutron reactions accounting for the multipliers of particle emission and the potential decay modes of the reaction products.

(6) In addition to the various types of output, all the multigroup response functions calculated by the code and/or supplied by the user can be obtained directly in the format of "MACK-Activity-Tables". These tables can be generated for the neutron energy groups only or for coupled neutron-gamma group structure and are directly usable with present transport codes.

This document is intended as a user's guide to MACK-IV. Attempts were made to make this document self-contained. However, the user may find it helpful to be generally aware of the contents of Ref. 1. Thorough knowledge of ENDF/B format is not required but some familiarity with this format is necessary for efficient utilization of MACK-IV. The rest of this document is organized as follows: Section II describes briefly the calculational methods in MACK-IV. Section III provides a description of the input instructions. Description of the output from MACK-IV is given in Sec. IV. Miscellaneous information about MACK-IV is given in Sec. V. Sample problems are given in Appendix A. In Appendix B, some information about ENDF/B files and reaction types are given.

II. CALCULATIONAL METHODS IN MACK-IV

The purpose of this section is to present the theoretical basis for the various types of calculations in MACK-IV. The neutron kerma factors are discussed in Part A, other response functions are described in Part B, and the gamma production cross sections are the subject of Part C.

A. Neutron Kerma Factors and Nuclear Heating

Calculation of the response function for nuclear heating commonly known as kerma factor is the central part of the MACK program. The basic theory for these calculations has been discussed previously in several documents (see for example Refs. 1 through 4). A summary of these theoretical bases is given in this subsection.

The nuclear heating $H_t(\vec{r})$, at any spatial point $\vec{r}$, is the sum of the neutron heating, $H_n(\vec{r})$, and the gamma heating, $H_\gamma(\vec{r})$, where[1-4]

$$H_n(\vec{r}) = \sum_j N_j(\vec{r}) \int \phi_n\left(\vec{r},E_n\right) k_{nj}\left(E_n\right)\, dE_n \,, \tag{1}$$

$$H_\gamma(\vec{r}) = \sum_j N_j(\vec{r}) \int \phi_\gamma\left(\vec{r},E_\gamma\right) k_{\gamma j}\left(E_\gamma\right)\, dE_\gamma \,, \tag{2}$$

and where $N_j(\vec{r})$ is the number density of nuclide j at $\vec{r}$; $k_{nj}\left(E_n\right)$ is the response function for nuclear heating which is more commonly known as the neutron kerma factor for nuclide j at neutron energy, E_n; $k_{\gamma j}\left(E_\gamma\right)$ is the gamma-ray kerma factor for nuclide j at photon energy, E_γ; and $\phi_n\left(\vec{r},E_n\right)$ is the neutron flux for neutrons of energy E_n. The gamma flux, $\left(\phi_\gamma\, r,E_\gamma\right)$ is obtained by solving the transport equation with a secondary photon production source,

$$S_\gamma\left(\vec{r},E_\gamma\right) = \sum_j N_j(\vec{r}) \int \phi_n\left(\vec{r},E_n\right) \sigma_{pj}\left(E_n,E_\gamma\right)\, dE_n \,, \tag{3}$$

where σ_{pj} is the photon production cross section in nuclide j for neutrons of energy E_n and photons of energy E_γ. The summation over j includes all nuclides in the mixture present at $\vec{r}$. The neutron kerma factor can be written as

$$k_{nj}(E) = \sigma_{tj}\left(E + \sum_{i}\frac{\sigma_{ij}}{\sigma_{tj}}Q_{ij} + \sum_{i'}\frac{\sigma_{i'j}}{\sigma_{tj}}E_{Di'j}\right.$$

$$\left. - \sum_{m}\frac{\sigma_{mj}}{\sigma_{tj}}\bar{E}_{n',mj} - \frac{1}{\sigma_{tj}}S_{E\gamma,j}\right), \qquad (4)$$

where σ_t is the total microscopic collision cross section, and the terms in parentheses are the energies contributed or taken by a particular reaction weighted by the relative probability of the reaction. The first term is the energy of the incident neutron times the probability that a collision occurred which is certain; Q_i is the energy resulting from mass conversion in reaction i; $E_{Di'}$ is the average decay energy per reaction i'; $E_{n',m}$ is the average secondary neutron energy per reaction m, and

$$S^{*}_{E\gamma,j}(E_n) = \int \sigma_{pj}(E_n,E_\gamma)E_\gamma \, dE_\gamma \, . \qquad (5)$$

The dependence of all terms in Eq. (4) on the incident neutron energy is obvious. The expression for gamma kerma factor can be written as

$$k_{\gamma j}(E) = \sigma_{pe,j} \cdot E + \sigma_{ca,j} \cdot E + \sigma_{pp,j} \cdot (E - a_{pp}) , \qquad (6)$$

where σ_{pe}, σ_{ca}, and σ_{pp} are the gamma-interaction cross sections for photoelectric, Compton absorption, and pair-production processes, respectively; and a_{pp} is equal to 1.02 MeV. The kerma factors are flux and density independent. The heating rate can therefore be calculated from neutron and photon transport results for any system if these factors are predetermined for all materials in the system. The evaluation of $k_{\gamma j}$ is straightforward and is normally performed by the codes which generate photon-interaction multigroup cross sections such as MUG.[5] Calculation of neutron kerma factors is complicated by the variety of reactions that a neutron can undergo, the kinematics for reactions in which more than one particle is emitted, and the demand for extensive nuclear data information.

All the terms in Eq. (4) except $S^*_{E\gamma}$ are calculated in MACK from basic nuclear data in files 1-5 of ENDF/B.[6] (See Table I.) The calculation of these terms is somewhat straightforward and is similar in many respects to the methodologies employed in other multigroup cross-section processing codes.[7-9] The calculation of $S^*_{E\gamma}$, however, is more involved and has been the subject of a large part of the developments in MACK-IV. This term can be calculated by the new version of the program MACK-IV via one of two paths as selected by the user:

Path I. The Direct Gamma-Production Path: In this path $S^*_{E\gamma}$ is calculated directly from the gamma-production data (files 12, 13, and 15 in ENDF/B, see Table I) according to Eq. (5).

Path II. The Indirect Gamma-Production Path: In this path the solutions of the kinematics equations (momentum and energy balance) of all nuclear reactions are used to calculate $S^*_{E\gamma}$. In this methodology no direct information on gamma production is required. One needs the individual neutron reaction cross sections and the energy and angular distributions in files 1-5 of ENDF/B. If charged particles are emitted in a reaction [e.g. (n,α) reaction], one needs the partial cross sections for this reaction to individual excited levels (i.e. the 700's MT series) or the energy distribution of the charged particles emitted. This type of information is scarce in ENDF/B and this leads to difficulties[3] in calculating neutron kerma factors for charged-particle-producing reactions associated with strong gamma-ray emission.

When energy-conserving gamma-production data are given in ENDF/B the gamma-production path provides a more reliable and straightforward methodology to calculating the neutron kerma factors. This path was not provided in the earlier version of MACK because of the lack of most gamma-production data at that time. These data have been provided for a large number of materials in ENDF/B-IV to warrant the new development. The nuclear kinematics (indirect gamma production) path has been retained and improved in MACK-IV because: (1) gamma-production data are still lacking for some important materials (e.g. ^{11}B, ^{232}Th, etc.); (2) the gamma-production data provided in ENDF/B for some materials are not consistent with the neutronics data content as to energy conservation; and (3) the kinematics path provides a convenient way for calculating the contribution to heating from each individual reaction, which is of interest in specialized nuclear and chemonuclear applications.

TABLE I

ENDF/B Files Processed by MACK-IV

File No. (MF)	Type of Data
1	General information
2	Resonance parameter data
3	Neutron cross sections
4	Angular distribution of secondary neutrons
5	Energy distribution of secondary neutrons
12	Multiplicities for photons (from neutron reactions)
13	Cross sections for photon production (from neutron reactions)
15	Energy distribution of photons (from neutron reactions)

We will attempt now to give some more details about the mechanics of calculating the neutron kerma factors in MACK-IV and also present some of the basic equations utilized. Equation (4) can be broken down into partial kerma factors representing the separate contributions of individual reactions. For simplicity, we will drop the subscript j designating a particular isotope (calculating kerma factor for mixtures of isotopes will be discussed later). In this case, we can write

$$k_n(E) = \sum_i k_{ni}(E) , \tag{7}$$

where $k_{ni}(E)$ is the neutron kerma factor for reaction i at an incident neutron energy E and is written as

$$k_{ni}(E) = \sigma_i(E) \cdot E_{Hi}(E) , \tag{8}$$

with σ_i as the reaction microscopic cross section at energy E and E_{Hi} is the part of the reaction energy deposited within a negligible distance from the site of collision. Thus E_{Hi} is the sum of the kinetic energies of the recoil nucleus and charged particles produced by the reaction. These charged particles include particles emitted directly such as an α-particle from (n,α) reaction as well as indirectly produced particles such as those from the internal conversion process. The contribution to energy deposition by charged particles emitted from radioactive decay of the reaction products is clearly time-dependent. However, since the decay energy decreases very rapidly with the lifetime of the radioactive nuclide and the concentration of short-lived isotopes generally reaches saturation in a relatively short time, the contribution to energy deposition from radioactive decay can be treated as time-independent and included in E_{Hi}. This assumption is, in general, reasonably accurate for steady-state systems provided that the radioactive nuclide does not have an unusually large transumation cross section. In Eq. (4) and in the following equation we add an energy deposition term representing the contribution from radioactive decay. The user of MACK, however, is allowed via the input options to include or exclude this term.

A general expression for E_{Hi} in any neutron reaction can be written from a simple energy balance

$$E_{Hi} = E + Q_i - E_{n'i} - E_{\gamma i} - E_i^* + E_{Di} . \quad (9)$$

In this equation Q is the Q-value of the reaction strictly defined as the difference in mass between the total mass of the reaction products and that of the neutron plus the target nucleus. E_n' is the total kinetic energy of all the neutrons emitted. E_γ is the total energy carried away with the gamma rays emitted. E^* is the (weighted) energy retained internally with any of the reaction products with a measurable lifetime as, for example, in the case of a recoil nucleus left in an isomeric state. In situations where E^* is non-zero one can treat the situation exactly or in a method similar to that used for E_D, i.e. assume $E^* = 0$ and adjust E_γ and E_D accordingly.

All the reaction products are emitted with energy and angular distributions. In calculating the nuclear heating, only an average over these distributions is required to yield energy deposition that is exact in the sense of a stochastic model. A bar will be used here over the appropriate parameters to indicate such averaging.

For convenience in treating the kinematics of neutron reactions, these reactions are grouped into the nine reaction types shown in Table II. To calculate the neutron kerma factors one needs the reaction cross sections, the Q-values, and the energies of the secondary neutrons and photons. The pointwise cross sections are processed from file 3 in ENDF/B and, for resonance-nuclides, are calculated in the resolved and unresolved resonance regions from resonance parameters in file 2 with an option for Doppler broadening. The Q-values are processed from file 3. The average kinetic energy of all secondary neutrons is calculated from the angular distribution in file 4 for elastic and inelastic level scattering and from the energy distributions given in file 5 of ENDF/B for other reactions. (See Table I and Appendix B for information on ENDF/B files and reaction numbers.) The calculations of the energy of the secondary photons is different in the direct (Path I) from that in the indirect path (Path II) as discussed earlier. In Path I, the $S_{E\gamma}^*$ in Eq. (4) is calculated directly by performing the integral in Eq. (5) once the gamma-production cross sections have been processed from files 12, 13, and 15 in ENDF/B as described later. The total energy carried away with all photons

TABLE II

Reaction Types

	Reaction Type	ENDF/B Reaction No., MT
(n,n)	Elastic	2
$(n,n')_\gamma$	Inelastic level	51-90
$(n,n')_\gamma$	Inelastic continuum	91
$(n,mn')a_{c_1}, a_{c_2}, \ldots$	(n,mn', charged particles), m = 1 or 2	22-24, 28-30, 32-36, and 51-91 with flag LR
$(n)a_{c_1}, a_{c_2}, a_{c_3}, \ldots$	(n, charged particles)	103-109 (700-799), 111-114
(n,γ)	Radiative capture	102
(n,2n)	Direct or level (n,2n)	16 and (6-9, 46-49)
(n,3n)	(n,3n)	17
(n,f)	Fission	18

from all reactions is calculated directly rather than by summing over gamma production for each individual reaction as this procedure assures better accuracy with the present status of the ENDF/B files. Therefore, with the direct gamma-production path (Path I), MACK-IV calculates only the total neutron kerma factor without calculating the neutron kerma factor for each individual reaction. In the indirect gamma-production path (Path II) the gamma energy is calculated separately for each reaction from expressions derived by applying linear momentum and energy conservation principles. Since the kinematics is similar for all reactions in each of the nine reaction types in Table I, the neutron kerma factor calculated by the indirect path are provided for each of these reaction types as well as for the total. In the following, we summarize some important equations for each of these reaction types concerning the calculation of the various terms in Eqs. (4) and (9).

Elastic Scattering

For elastic scattering, all terms on the right-hand side of Eq. (9) are zero except the incident neutron energy and the kinetic energy of the neutron emitted. The latter is simply

$$\bar{E}_{n'} = E \frac{A^2 + 1 + 2A\bar{\mu}_{cm}}{(A + 1)^2} , \tag{10}$$

where A is the ratio of the nuclear mass of the nuclide to that of the neutron and $\bar{\mu}$ is the average of the cosine of the center-of-mass scattering angle,

$$\bar{\mu}_{cm} = \overline{\cos \theta_{cm}}$$

and

$$\bar{\mu} = f_1 , \tag{11}$$

with f_1 as the first coefficient of the Legendre polynomial expansion of the differential scattering probability distribution ($f_0 = 1$).

Inelastic-Level Scattering

For inelastic-level scattering $(n,n')\gamma$, Q = 0, and $\bar{E}_{n'}$ and $\bar{E}_{\gamma}$ are derived as follows:

$$\bar{E}_{n'}(E) = \frac{2AE}{(A+1)^2}\left[\frac{A^2+1}{2A} - \frac{A+1}{2E}\cdot E_\lambda + \left(1 - \frac{A+1}{A}\frac{E_\lambda}{E}\right)^{1/2}\bar{\mu}_{cm}\right], \quad (12)$$

where

E_λ = energy of the excited level

$\bar{\mu}_{cm} = \overline{\cos\theta_{cm}}$.

The average of the cosine of the scattering angle in the center-of-mass is evaluated from the secondary neutron angular distribution in file 4 of ENDF/B. This angular distribution can be given in either

(1) Lengendre coefficients in the center-of-mass (CM) system;

(2) tabulated normalized probability distribution in the CM, $P_{cm}(\mu,E)$;

(3) Legendre coefficients in the laboratory (LAB) system; and

(4) tabulated normalized probability distribution in the LAB system, $P_{LAB}(\mu,E)$.

For case (1), $\bar{\mu}_{cm}$ is equal to the first coefficient (f_1) of the Legendre polynomial expansion ($f_0 = 1$). In case (2),

$$\bar{\mu}_{cm}(E) = \int_{-1}^{+1} \mu P_{cm}(\mu,E)\, d\mu \ . \quad (13)$$

For cases (3) and (4) a transformation from the LAB to the CM system is performed and $\bar{\mu}_{cm}$ is calculated. Another procedure is to replace Eq. (12) with the following:

$$\bar{E}_{n'}(E) = E\left\{\frac{1}{A+1}\bar{\mu}_L + \left[\frac{A-1}{A+1} + \frac{1}{(A+1)^2}\overline{\mu_L^2} - \frac{A}{A+1}\frac{E_\lambda}{E}\right]\right\}^2 , \quad (14)$$

where μ_L is the cosine of the LAB scattering angle. $\bar{\mu}_L$ can be evaluated as the first coefficient of the Legendre polynomial expansion in the LAB system or from $P_{LAB}(\mu,E)$ as in Eq. (13). $\overline{\mu_L^2}$ can be evaluated as follows:

$$\overline{\mu_L^2} = \frac{1}{3}(1 + 2f_2) , \tag{15}$$

where f_2 is the second coefficient of the Legendre polynomial expansion in the LAB system. For case (4),

$$\overline{\mu_L^2} = \int_{-1}^{+1} \mu^2 P_{LAB}(\mu,E)\, d\mu . \tag{16}$$

The gamma energy is calculated directly from the ENDF/B gamma production files for Path I. In Path II, it is given by

$$\bar{E}_\gamma = \frac{1}{1 + C_F} E_\lambda , \tag{17}$$

C_F = internal conversion factor

Inelastic Scattering, $(n,n')\gamma$ to the Continuum

In this case Q = 0. The average kinetic energy for the secondary neutron is calculated from the secondary neutron energy distribution in file 5 of ENDF/B. This energy distribution, $P(E \to E')$, can be broken down into partial energy distributions, $f_k(E \to E')$, where each of the partial distributions can be described by a different analytic representation:

$$P(E \to E') = \sum_{k=1}^{NK} P_k(E) f_k(E \to E') ,$$

and at a particular incident neutron energy E,

$$\sum_{k=1}^{NK} P_k(E) = 1 .$$

The ENDF format allows several analytic formulations for the partial energy distributions, $f_k(E \to E')$.

An expression for $\overline{E_{n'}}$ is evaluated as follows:

$$\bar{E}_{n'}(E) = \frac{\int_{E'_{min}}^{E'_{max}} E'P(E \to E')\, dE'}{\int_{E_{min}}^{E'_{max}} P(E \to E')\, dE'}$$

$$= \sum_{k=1}^{NK} P_k(E) \int_{E'_{min}}^{E'_{max}} E' f_k(E \to E')\, dE'$$

$$= \sum_{k=1}^{NK} P_k(E) \bar{E}_{n',k} \,. \tag{18}$$

The analytic form of $\bar{E}_{n',k}$ depends on the analytic formulation of $f_k(E \to E')$.

For the evaporation spectrum

$$f(E \to E') = \frac{E'}{I} \exp[-E'/\theta(E)] \,,$$

where I is a normalization constant that depends on E'_{min}, E'_{max}, and θ. The ENDF assumes that $E'_{min} = 0$. Using this assumption, we obtain

$$\bar{E}_{n',k} = \theta \frac{2 \exp(x_1) - [1 + (1 + x_1)^2]}{\exp(x_1) - (1 + x_1)} \,, \tag{19}$$

where

$$x_1 = \frac{E'_{max}}{\theta} \,.$$

For a simple fission spectrum (Maxwellian),

$$f(E \to E') = \frac{\sqrt{E'}}{I} \exp[-E'/\theta(E)] \,, \tag{20}$$

and by invoking the assumption that $E'_{min} = 0$, we obtain

$$\bar{E}_{n',k} = \theta \left\{ \frac{3}{2} - \frac{x_1^{3/2}}{[(\sqrt{\pi}/2)\exp(x_1)\mathrm{erf}(\sqrt{x_1}) - \sqrt{x_1}]} \right\} . \qquad (21)$$

A similar expression can be derived for the Watt spectrum. For the other allowable representations of $f_k(E \rightarrow E')$, $\bar{E}_{n'}$ can be obtained by numerical integration in Eq. (18). $\bar{E}_\gamma$ can be evaluated directly from the gamma energy distribution in Path I. In Path II, applying the equations for conserving linear momentum and energy balance and assuming that neutrons are emitted isotropically in the center-of-mass system, one can derive the following expression for the average excitation energy, $\bar{\varepsilon}$, of the residual nucleus following the emission of the neutron,

$$\bar{\varepsilon} = \frac{A^2 + 1}{A(A + 1)} E - \frac{A + 1}{A} \bar{E}_{n'} . \qquad (22)$$

$\bar{E}_\gamma$ is equal to $\bar{\varepsilon}$ unless internal conversion is significant in which case

$$\bar{E}_\gamma = \frac{1}{1 + C_F} \bar{\varepsilon} . \qquad (23)$$

(n,2n) Reaction

The (n,2n) reaction can currently be represented in ENDF/B as direct (n,2n) (MT = 16) and/or as a time-sequential reaction (MT = 6-9; 46-49). In the time-sequential (n,2n) reaction, $A(n,n_1)A^*(n_2)(A - 1)^*$, the first neutron is essentially an inelastic scattering event that may leave the nucleus A^* in one of several excited states. The second neutron is subsequently emitted by the decay of the recoiling nucleus A^*. The kerma factor for the (n,2n) reaction is obtained by summing the contribution from the direct and each sequence (defined by an excited level of A^*) of the time-sequential reactions.

For direct- and time-sequential (n,2n), Eq. (9) is applicable with the Q-value as the binding energy B, of the last neutron in the target nucleus and $\bar{E}_{n'}$ as the average of the sum of the kinetic energies of the two neutrons. For the direct (n,2n)(MT = 16), $\bar{E}_{n'}$ can be evaluated from the secondary neutron energy distribution given in file 5 of ENDF/B as described under inelastic scattering to continuum. For each of the time-sequential reaction, the energy of the excited level in A^* is known and the average kinetic energy of the first

neutron is calculated from the angular distribution in file 4 of ENDF/B according to Eq. (12). The average kinetic energy of the second neutron is calculated from the energy distribution in file 5 of ENDF/B.

If the direct gamma-production path is not selected, the average energy of the photons emitted [E_γ in Eq. (9)] can be calculated from momentum and energy balance. The results are different for direct (n,2n) from those for time-sequential (n,2n). For direct (n,2n), assuming isotropic emission in the center-of-mass, the excitation energy of the residual nucleus is given by [in the direct (n,2n) the time interval between the emission of the two neutrons is so short that the intermediate nucleus A^* does not deposit any of its recoil energy prior to the second neutron emission]

$$\bar{\varepsilon}_{A-1} = \frac{A^2 + 2}{A(A+1)}E - \frac{1}{A-1}\left[\frac{A^2 - 2}{A}\overline{E_{n'1}} + A\,\overline{E_{n'2}}\right] - B \,. \qquad (24)$$

where $\bar{E}_{n'1}$ and $\bar{E}_{n'2}$ are the average energies of the first and second neutrons. At present, ENDF/B provides only the combined spectrum of the two neutrons; and therefore evaluating Eq. (24) requires invoking the assumption that $A^2 >> 2$.

For a sequence (e.g. MT = 6 and 46) in a time-sequential (n,2n) reaction, it is assumed that the intermediate nucleus A^* comes to rest prior to emission of the second neutron. Thus, the excitation energy of the residual nucleus is given by

$$\bar{\varepsilon}_{A-1} = E_\lambda - B - \frac{A}{A-1}\bar{E}_{n2} \,, \qquad (25)$$

where E_λ is the energy of the excited level in A^* and $\bar{E}_{n2}$ is the average energy of the second neutron.

Notice that ^{8}Be formed from the (n,2n) reaction in ^{9}Be eventually decays with an extremely short half-life into two alpha particles with a decay energy of 0.095 MeV. MACK checks the atomic and mass numbers of materials to allow for special treatments. For ^{9}Be(n,2n), MACK assumes that the excitation energy $\bar{\varepsilon}_{A-1}$ is deposited locally by the alpha particles rather than carried away with gamma rays.

(n,3n) Reaction

Equation (9) applies here with the Q as the Q-value of the (n,3n) reaction and $\bar{E}_n$, as the average of the sum of the kinetic energies of the three neutrons. The latter is calculated from the secondary neutron energy distribution. The energy of the photons emitted is calculated in the indirect gamma-production path from the excitation energy of the residual nucleus. This can be calculated by applying linear momentum and energy balance. For direct (n,3n) the time interval between neutron emissions can be assumed to be extremely short. Assuming isotropic neutron emission in the center-of-mass system, the excitation energy of the residual nucleus can be derived as

$$\bar{\varepsilon}_{A-2} = \frac{A^2 + 3}{A(A + 1)} E + Q_{n3n} - \left[\frac{A^2 - 3}{A(A - 1)} \bar{E}_{n1} + \frac{A^2 - 2A - 1}{(A - 1)(A - 2)} \bar{E}_{n2} + \frac{A - 1}{A - 2} \bar{E}_{n3}\right], \quad (26)$$

where Q_{n3n} is the Q-value of the (n,3n) reaction (always negative) and $\bar{E}_{n1}$, $\bar{E}_{n2}$, and $\bar{E}_{n3}$ are the average kinetic energies of the first, second, and third neutrons. Since ENDF/B provides only the combined spectrum for the three neutrons, invoking the assumption that $A \gg 1$ is necessary for evaluating the above expression.

Radiative Capture

In an (n,γ) reaction, conservation of linear momentum causes the kinetic energy of the residual nucleus to be very small; in general; only a fraction of 1% of the energy of the emitted photons. The energy $\bar{E}_\gamma$ of the photons emitted can be derived as

$$\bar{E}_\gamma = M_r C^2 \left\{\sqrt{1 + \frac{2}{M_r C^2}\left[Q + E\left(1 - \frac{m_n}{M_r}\right)\right]} - 1\right\}. \quad (27)$$

The recoil energy of the nucleus, $\bar{E}_r$, is

$$\bar{E}_r = E + Q - \bar{E}_\gamma , \quad (28)$$

where

Q = the reaction Q-value

$M_r C^2$ = mass of the residual nucleus in energy units

$M_r C^2 = (A + 1)m_n C^2 - Q$

$m_n C^2$ = energy equivalent of the neutron mass (939.512 MeV)

Charged Particle Reactions

The reaction discussed here is of the type

$$ {}_{Z_1}X^{A_1}\left(n;\ a_{c_1} a_{c_2} \ldots a_{c_n}\right) {}_{Z_2}Y^{A_2} \ , $$

where a_{c_1}, a_{c_2} . . . are charged particles, e.g. (n,α), (n,p), (n,αT). The energy deposited, E_H per reaction as defined in Eq. (9), is the sum of the kinetic energies of the recoil nucleus and charged particles emitted, i.e.

$$ E_H = E_r + E_{a_{c_1}} + E_{a_{c_2}} + \ldots + E_{a_{c_n}} = E + Q - \bar{E}_\gamma \ , \qquad (29) $$

where Q is the reaction Q-value (mass difference) and $\bar{E}_\gamma$ is the average energy emitted with the photons. The residual nucleus is frequently left in one of the excited states. If we define the cross section for the i-th excited state as σ_i, then the total reaction cross section σ is

$$ \sigma = \sum_{i=0}^{N} \sigma_i \qquad (30) $$

and the total kerma factor for the reaction is

$$ k = \sigma\left[E + Q - \bar{E}_\gamma + \bar{E}_D\right] \ , \qquad (31) $$

where

$$\bar{E}_\gamma = \sum_{i=0}^{N} P_i \varepsilon_i \ , \tag{32}$$

$$\bar{E}_D = \sum_{i=0}^{N} P_i E_{Di} \ ; \tag{33}$$

ε_i = energy of the i-th level ($\varepsilon_0 = 0$)

E_{Di} = contribution to energy deposition by radioactive decay of the i-th level

P_i = probability that the i-th level will be excited given that a reaction has occurred (σ_i/σ).

If other processes compete with gamma emission (e.g. interval conversion), the ε_i's in the above expressions should be adjusted.

The reaction total cross section and Q-value for (n, charged particle) reactions are given in ENDF/B with MT = 103-107. The corresponding partial cross sections to various excited states are given in the MT = 700-799 series. For many materials, however, the 700's series data are not given. In such cases (and for MT = 108-114), there is presently no method to calculate $\bar{E}_\gamma$ in Eq. (32) for the limited information given in files 1-5. This is the basic disadvantage of the indirect gamma-production path. The newly proposed format for including the energy distribution of the charged particles can help solve this problem. In practice, however, data on gamma-production and charged-particle energy are both either lacking or both are known.

(n,n') Charged Particles

This reaction is generally of the form

$$_{Z_1}X^{A_1}(n,n')\ a_{c_1},\ a_{c_2},\ \ldots\ a_{c_n},\ _{Z_2}Y^{A_2} \ .$$

The energy deposition per reaction E_H is the sum of the kinetic energies of the recoil nucleus and charged particle emitted and its calculation from Eq. (9) depends on the type of data available.

In ENDF/B, some of these (n,n') charged particle reactions are represented in the format of inelastic level scattering, (n,n'x) (MT = 51-90) with an LR flag to define the exact type of the reaction. For such type of reaction, two Q-values are given; SQ is the Q-value for the combined (n,n'x) reaction and Q' is the energy of the excited level for the (n,n') part of the reaction. The energy of the secondary neutron can thus be evaluated from Eq. (12) with $E_\lambda = |Q'|$ and the angular distribution of the secondary neutron in file 4. Therefore, with this type of format the (n,n') charged particle reaction can be treated as inelastic level scattering except for the following differences: (1) the Q-value for the reaction is SQ instead of zero; and (2) the energy available to the gamma rays in inelastic level scattering are taken by the charged particles and deposited locally.

The flags LR = 39 and LR = 40 are also used in ENDF/B to indicate that the final mode of decay of the residual nucleus from an (n,n') reaction is by internal conversion (LR = 39) or by electron position pair formation (LR = 40). These two cases are treated similar to the (n,n') charged particle reactions except that 1.02 MeV of energy is carried away with photons in the case of the electron-positron formation mode and is not available for local energy deposition.

The (n,n') charged particle reactions can also be given in ENDF/B as direct (composite) reactions (e.g. MT = 22, 23, etc.). Also, this is always the case for the (n,2n) charged particle reactions (e.g. MT = 24). In these cases, the average energy of the secondary neutron [Eq. (9)] is calculated from the energy distribution of file 5. The information in the neutronics files (1-5), however, is not sufficient to calculate the energy carried away with the emitted gamma rays. This difficulty is similar to that discussed earlier for the (n, charged particles) reactions.

The Fission Reaction

Despite the extensive theoretical and experimental work on fission, there are still considerable uncertainties in the magnitude of energy deposition by the products of the fission reaction. These uncertainties are largest

for high incident-neutron energies. The general equation, Eq. (9), for energy deposition is also applicable to fission but some elaboration is necessary.

The fission of a nucleus of mass number A and atomic number Z with a neutron of an incident neutron energy E can be written[10] as

$$(A,Z) + n + E_i \rightarrow \left(A_L + Z_L\right) + \left(A_H + Z_H\right) + \nu n' + \gamma's + \beta's + \nu^*'s + E_K + E_{n'} + E_\gamma + E_\beta + E_{\nu^*} , \quad (34)$$

where subscripts L and H denote respectively light and heavy stable fission products, $\bar{\nu}$ is the number of prompt and delayed neutrons emitted, n, γ, β, and ν^* refer respectively to a neutron, photon, beta-particle, and antineutrino. $E_K = E_L + E_H$ is the total kinetic energy of the fission fragments, $E_{n'}$ is the total kinetic energy of the emitted prompt and delayed neutrons, E_γ, E_β, and E_{ν^*} are the kinetic energies of the emitted photons, beta particles, and anti-neutronios, respectively. The Q-value for fission (defined as the mass difference consistent with other reactions considered previously) is

$$Q = M(A,Z) - \sum_i y_i M\left(A_i,Z_i\right) - (\bar{\nu} - 1)m_n , \quad (35)$$

where $\left(A_i,Z_i\right)$ is the i-th stable fission product of yield y_i, m_n is the neutron mass; all masses are in energy units. The total energy available to the fission reaction is $E_i + Q$ which is equal to the total energy of the products of the fission reaction.

$$E_i + Q = \bar{E}_K + \bar{E}_{n'} + \bar{E}_\gamma + \bar{E}_\beta + \bar{E}_{\nu^*} , \quad (36)$$

where the bars denote averages over all fission modes. Notice that E_K here refers to the post-neutron emission value.

According to our earlier definition of the neutron kerma factor, $k = \sigma_f E_{Hf}$ where σ_f is the fission cross section and E_{Hf} is the local energy deposition as defined in connection with Eq. (8). It follows from this definition that $E_{Hf} = \bar{E}_K$, i.e. the average kinetic energy of the final fission fragments. If radioactive decay is to be accounted for as an approximate steady-state term, then $E_{Hf} \simeq \bar{E}_K + \bar{E}_\beta$. Therefore, one can write for the fission reaction an expression for E_H similar to that of Eq. (9), i.e.

$$E_{Hf} = \bar{E}_K = E_i + Q - \bar{E}_{n'} - \bar{E}_\gamma - E_{\nu^*} - \bar{E}_\beta \qquad (37a)$$

or, if radioactive decay is to be approximately included:

$$E_{Hf} = \bar{E}_K + \bar{E}_\beta = E_i + Q - \bar{E}_{n'} - \bar{E}_\gamma - E_{\nu^*} \, . \qquad (37b)$$

The local energy deposited per fission reaction, E_{Hf}, can be calculated directly from information on $\bar{E}_K$ or by evaluating the right-hand side of Eq. (37). At present, there is no provision in ENDF/B format to directly evaluate $\bar{E}_K$ as a function of the incident neutron energy. A problem with evaluating the right-hand side of Eq. (37) is in the definition of Q. In the past, the Q-value for fission (as for all the Q-values in ENDF/B, no energy dependence is provided) has been defined in several ways for different material evaluations. With the definition presently favored in ENDF as $Q_{ENDF} = Q - E_{\nu^*}$ evaluation of the right-hand side of Eq. (37) can be easily performed without difficulty except for cases where the energy dependence of Q (and E_β) is important.

In MACK-IV we have chosen not to limit the user to any particular treatment of the energy deposition in the fission reaction. One strong reason for this is that previous conclusions from evaluations (e.g. Ref. 10-12) for thermal and fast reactors may not be valid in other applications such as the fusion hybrid where the dependence[12] of the energies of the products from fission on incident neutron energy can be significant. As shown later in this report, MACK-IV permits the user to have control via the input on how the neutron kerma factor for the fission reaction is calculated. One should note, in passing, that the user of MACK-IV need not worry in evaluating energy deposition for fissionable materials about the approximations previously[11] employed for reactions other than fission. The kerma factor for all reactions are calculated accurately for fissionable as well as nonfissionable materials.

Kerma Factors for a Mixture of Isotopes[1,2]

The kerma factors for a mixture of isotopes can be obtained by summing the macroscopic kerma factors for all isotopes present in the mixture. For example, consider an element or a mixture which consists of several isotopes. The kerma factor for the mixture is

$$K_m = \sum_j K_j \ , \tag{38}$$

and

$$K_j = N_j k_j \ , \tag{39}$$

where

k_j = microscopic kerma factor for the j-th isotope in the mixture

N_j = number density of the j-th isotope in the mixture

K_m = macroscopic kerma factor for the mixture.

It may be desirable for some natural elements (e.g. molybdenum, iron, etc.) which consist of several isotopes to evaluate directly the kerma factors for the element without calculating the K_j's. This requires appropriate definitions of the various physical quantities involved in kerma calculations. The guiding rule is that the definitions of the physical quantities and the equations for K_m must reproduce Eq. (38). A definition of the Q-value for a mixture of isotopes is discussed below.

Consider a reaction which occurs in one or more of these isotopes, and consider the definition

$$\text{Q-value for the j-th isotope} = Q_j = E_{R_j} - E \ , \tag{40}$$

where E_{R_j} is the kinetic energy of the product particles and E is the kinetic energy of the colliding particles. Since the kinetic energy released in the mixture must equal the sum of the kinetic energies released in the various isotopes in the mixture, we can write

$$N_m \sigma_m E_{R_m} = \sum_j N_j \sigma_j E_{R_j} \ , \tag{41}$$

where E_{R_m} is the kinetic energy of the product particles per reaction in the mixture. Making use of the definitions of Q_j and σ_m which is

$$\sigma_m = \sum_j \frac{N_j \sigma_j}{N_m} ,$$

we can write Eq. (41) as

$$E_{R_m} - E = \sum_j Q_j \frac{\sigma_j N_j}{\sigma_m N_m} . \tag{42}$$

Since the left-hand side of Eq. (42) is the kinetic energy released by or required for a reaction in the mixture, the right-hand side is recognized as the Q-value for the mixture, i.e.,

$$Q_m = \sum_j Q_j \frac{\sigma_j N_j}{\sigma_m N_m} . \tag{43}$$

Since definition (43) is derived by using only a conservation principle Eq. (41) and the basic definition of the Q-value for an isotope, it is a unique definition compatible with the definition of the Q-value for an isotope; and it should be acceptable for all physics calculations that use the Q-value in its normal definition.

Similar definitions for the various physical quantities for a mixture of isotopes can be easily developed by applying similar arguments. For example, the average energy of a secondary neutron from a reaction in the mixture and the decay energy can be written as

$$\bar{E}_{n',m} = \sum_j \frac{N_j \sigma_j}{N_m \sigma_m} \bar{E}_{n',j} , \tag{44}$$

and

$$E_{decay,m} = \sum_j \frac{N_j \sigma_j}{N_m \sigma_m} E_{decay,j} . \tag{45}$$

Writing an equation for the kerma factor for any reaction in a mixture in the same form as for a single isotope with the physical quantities involved

as defined above, it is easy to see that it satisfies Eq. (38). This is no surprise since kerma itself is a physical quantity and Eq. (38) is merely an expression for a physical conservation law. In other words, any definition of the physical quantities for a mixture of isotopes that satisfies the physical laws (e.g. energy and momentum conservation) would necessarily be compatible with Eq. (38).

A special case implicitly included in Eqs. (43)-(45) is a reaction which occurs only in one isotope. In this case Eq. (44) reduces to

$$\bar{E}_{n',m} = \bar{E}_{n',j} ,$$

where J is the isotpe in which this reaction occurs. An example is inelastic-level scattering where each level belongs to a particular isotope. Therefore, in applys Eqs. (12) and (14) for a mixture of isotopes, A should be taken as the atomic weight ratio for the particular isotope in which the level considered is excited.

From the above discussion, it can be seen that for single isotopes energy-independent parameters such as the Q-values, decay energies, etc., are energy-dependent for a mixture of isotopes because σ_j/σ_m is generally energy-dependent for any reaction except the special case of a reaction that occurs only on one isotope.

Another observation worth making is that kerma calculations cannot be accurately made if nuclear data is available only for the mixture and not for the constituent isotopes. For example, the use of only an abundance-weighted Q-value for a reaction such as (n,p) would result in a negative kerma factor for that reaction in an energy range whose width depends on the thresholds of the reaction and constituent isotopes.

Energy Deposition Due to Radioactive Decay

As discussed earlier, particle emission from the decay of the activated residual nuclei must be considered in the calculation of neutron kerma factors as it is another mechanism for local energy deposition. Since radioactive decay is time dependent, the kerma factors for nuclear reactions followed by radioactive decay is time dependent.

However, the most important contribution to energy deposition from radioactive decay is generally from short-lived residual nuclei since the mean lifetime for decay decreases rapidly as the disintegration energy increases. The contribution from activated residual nuclei with a mean lifetime greater than a few days is usually negligibly small. Thus, kerma factors in which radioactive decay is considered only for half lives less than an arbitrary cutoff (e.g. 10 days) is suitable for steady-state heating rate calculations provided that the rate of transmutation of the radioactive isotope is small. If the heating rate is to be calculated for a short period of operation of the nuclear system (e.g. startup), then the contribution from radioactive decay should be calculated separately from the contribution to energy deposition by charged-particle recoil from nuclear reactions. Clearly, the latter is always time-independent (energy release, not heating rate).

The most frequent type of decay is by emission of beta particles. β^+ decay may occur after (n,2n) reactions and β^- after (n,γ) and (n, charged particles) reactions. Since beta particles are emitted with an energy spectrum, the average kinetic energy of beta particles, $\bar{E}_\beta$ must be calculated.

References 1 and 2 discuss a method for evaluating $\bar{E}_\beta$ for β^+ and β^- as a function of the end-point energy for the beta particle and the atomic number of the nucleus. The tables in Ref. 1 should be consulted for recommended values of $\bar{E}_\beta$.

B. Reaction Cross Sections and Other Response Functions

In addition to the neutron kerma factors, MACK-IV calculates the multigroup cross sections for important reactions and the multigroup response functions for helium, hydrogen, and tritium production. The code permits other response functions, e.g. atomic displacement cross sections and gamma kerma factors, to be included in input; these together with the response functions generated internally in the code are outputted in several modes (print, punch, tape). One of the most important modes of output is the MACK-Activity-Tables. As described later in the input and output instructions, these tables can be used directly with transport codes to calculate the rates of nuclear responses. The format of this activity table is shown in Table III.

TABLE III

MACK-Activity Table

Position	Content
1	Neutron and gamma kerma factors
2	Neutron kerma factor
3	Gamma kerma factor
4	Displacement cross section - A
5	Displacement cross section - B
6	Total hydrogen production cross section
7	Total tritium production cross section
8	Total helium production cross section
9	Total cross section
10	Elastic cross section
11	Total inelastic cross section
12	Total (n,2n) cross section
13	(n,3n) cross section
14	Total fission cross section
15	(n,n't) cross section
16	(n,n') continuum cross section
17	(n,γ) cross section
18	(n,p) cross section
19	(n,D) cross section
20	(n,t) cross section
21	(n,^{3}He) cross section
22	(n,α) cross section
23	Elastic scattering kerma factor
24	(n,n') charged particles kerma factor
25	Inelastic-level scattering kerma factor
26	(n, charged particles) kerma factor
27	(n,2n) kerma factor
28	(n,3n) kerma factor
29	Fission kerma factor
30	Inelastic continuum kerma factor
31	Radiative capture kerma factor
32	Group mid-energy for neutron and gamma
33	Group mid-energy for neutron only
34	Group mid-energy for gamma only
35	Positions 35 through IHM are filled with cross sections for the MT reactions not given in the fixed positions 1 through 34.
.	
.	
.	
IHM	

The pointwise cross sections are calculated from file 3 in ENDF/B except for resonance materials where resonance parameters are provided in file 2. For resonance materials, the cross sections for total, elastic, fission, and radiative capture are calculated by the code in the resolved and unresolved resonance regions from the resonance parameters in file 2 and combined with the background cross sections in file 3. The code provides an option for Doppler broadening of the cross sections in the resonance region. An option is also provided in the code to read the cross sections for resonance materials from an input tape generated from a previous MACK run or by other processing codes.[7-9]

The multigroup cross sections are generated from the pointwise cross sections using a weighting function selected by the user from several built-in functions or provided as an input. Response functions for helium, hydrogen, and tritium productions are calculated by summing the production cross sections for the appropriate reactions where the production cross section for a reaction is the reaction cross section times the multiplicity of emission for the particle of concern. For example, the helium-production cross section is equal to $\sigma(n,\alpha) + \sigma(n,n'\alpha) + 2\sigma(n,2\alpha) + 2\sigma(n,n'2\alpha) + 3\sigma(n,3\alpha) + 2\sigma(n,d2\alpha) + \ldots$, etc. Other information about response functions is provided in the input and output sections.

C. Gamma Production

The gamma-production files (12-15) in ENDF/B are processed to calculate one or more of the following: (1) the total energy carried away with the photons emitted in a neutron-induced reaction [$S^*_{E\gamma}$ in Eq. (5) or $\bar{E}_\gamma$ in Eq. (9)]; (2) the gamma-production cross-section matrix, $\sigma_p\left(E_n,E_\gamma\right)$; and (3) the gamma-energy-production matrix, $E_\gamma\sigma_p\left(E_n,E_\gamma\right)$. The first quantity $S^*_{E\gamma}$ or $\bar{E}_\gamma$ is needed for calculation of the neutron kerma factors by the direct gamma-production path discussed earlier in this section. The gamma-production number and energy cross sections are by-products of the calculation of the first quantity and are outputted by the code if the user selects the appropriate input options.

The gamma-production data given in file 12 are multiplicities and transition probability arrays. Multiplicities are used to represent the cross sections of discrete photons and/or the integrated cross sections of continuous

photon spectra. The transition probability arrays are used to represent the discrete gamma when the energy levels are known. Both of these representations require the neutron data cross sections from the neutron data files. File 13 gives the photon-production cross section in absolute way, i.e. no need for neutron cross sections from the neutron data files. File 15 provides the photon energy spectra for the continuum data given in files 12 and 13.

III. INPUT DESCRIPTION

Part A of this section provides the input instructions for MACK-IV. The user is expected to refer to this part often in the process of preparing the input. Therefore, the instructions in this section are kept brief. Other detailed information given in Part B and elsewhere in this report should help the user make a correct interpretation of the input instructions.

A. Input Instructions

The set of cards specified in the following instructions is required for each material. Computations can be made for as many materials as desired in a single run by simply repeating this set of cards for each material desired. The ENDF/B data does not have to be on the same tape for all materials provided that the logical unit for the ENDF/B tape and the rewinding options (specified in the following input instructions) are specified correctly. No rewind operations are performed on the output files inbetween processing of different materials. The rewind operation is invoked only after processing the last material in a run.

CARD NO. 1 FØRMAT (18A4)

Title card used as a heading for the different sections of the output for a material.

CARD NO. 2 FØRMAT (4A4,2X,9I6)

MATHØL	Material name (16 characters)
MATNØ	ENDF/B material number (MAT number)
NDFB	Logical unit number for ENDF/B data tape (default = 10)
IDTAP	ENDF/B TAPE identification number
MØDE	Mode of ENDF/B data file 1 = binary tape 2 = BCD tape
IREW	0 = No effect 1 = Rewind the ENDF/B data tape before beginning the search for this material

IRESØN	0 = No effect 1 = Calculate resonance cross sections if resonance parameters are present (in file 2 of ENDF/B) 2 = Read resonance cross sections from input data set on logical unit IØ17
NEP	Number of energy points used for energy mesh
NGRPS	Number of neutron energy groups
IØ17	Logical unit for resonance cross sections (default = 17)

CARD NO. 3 FØRMAT (12I6)

This data card is required only if IRESØN = 1

NSIGP	Number of σ_0 values (maximum 7)
JWRIT	0 = No effect 1 = Print resonance cross sections (can be very lengthy printout)
IRINTG	0 = No effect 1 = Calculate the resonance integral

CARD NO. 4 FØRMAT (6E12.4)

This data card is required only if IRESØN = 1

EPS	The relative accuracy which is used for the resonance calculations. The resonance routines process resonance ENDF nuclides and generate point files for the total, fission, elastic, and (n,q) cross sections. These files are similar to file 3 of an ENDF library. The resonance routine eliminates the unncessary points from TAB1 record if they can be predicted by interpolation between adjacent points with relative accuracy better than EPS. (The default value for EPS is 0.001.)
RFACT	The resolved resonce region energy mesh is based on this parameter. The energy points are chosen such that the ratio of total cross section from point to point is roughly RFACT. (The default value for RFACT is 0.9.)
SFACT	Number of practical widths over which the RFACT scheme is used for a particular resonance. (The default value for SFACT is 10.0.)
TDEGK	Temperature in degrees kelvin for Doppler broadening. (Default = 300)

CARD(s) NO. 5 FØRMAT (6E12.4)

This may be one or two cards and is entered only if IRESØN = 1 and NSIGP $\geq$ 1.

SIGIN(1) SIGIN(2) . . . SIGIN(NSIGP)	σ_0 array for the unresolved resonance calculation. σ_0 is the potential scattering cross section in barns per atom of the resonance nuclide for nuclide which is mixed with the resonance nuclide. The σ_0 values should be input high to low. (A value of 10^8 is recommended for SIGIN(1)).

CARD NO. 6 FØRMAT (3I6,2E12.4)

This data card is required only if IRESØN = 2 to provide the instructions for reading the user's resonance cross-section tape.

NRST	Number of MT reactions on the tape
MAXN1	TAB1 array length for NBT, JNT
MAXN2	TAB1 array length for x, y
ELØR	The lowest energy for the resonance region
EHIR	The highest energy for the resonance region

CARD NO. 7 FØRMAT (12I6)

LINK1A	0 = No effect 1 = Process pointwise cross sections
LINK1B	0 = No effect 1 = Calculate group cross sections (LINK1A must be 1)
LINK2A	0 = No effect 1 = Calculate pointwise kerma factors (LINK1A must be 1)
LINK2B	0 = No effect 1 = Calculate group kerma factors (LINK2A must be 1)
IPRT1A	0 = No effect 1 = Print pointwise cross sections
IPRT1B	0 = No effect 1 = Print group cross sections

IPRT2A

0 = No effect

1 = Print pointwise kerma factors by reaction

2 = Write pointwise kerma factors by reaction (and total) on tape

3 = Both 1 and 2

4 = Write only pointwise total kerma factor on tape (the total kerma factor is always printed)

IPRT2B

0 = No effect

1 = Print group kerma factors

IPUN1A

0 = No effect

1 = Punch pointwise cross sections except for MT = 51 to 90 and 700 to 799

2 = Punch pointwise cross sections except for MT = 700 to 799

3 = Punch printwise cross sections for all reactions

IPUN1B

-3 = Write group reaction cross sections on tape for all reactions

-2 = Write group reaction cross sections on tape for all reactions except for MT = 700 to 799.

-1 = Write group reaction cross sections on tape for all reactions except for MT = 51 to 90 and MT = 700 to 799.

0 = No effect

1 = Punch group reaction cross sections for all reactions except for MT = 51 to 90 and 700 to 799

2 = Punch group reaction cross sections for all reactions except for MT = 700 to 799

3 = Punch group reaction cross sections for all reactions

IPUN2A

0 = No effect

1 = Punch pointwise kerma factor by reaction and total (for MLINK2 $\neq$ 2 only total is available)

2 = Punch pointwise total kerma factor

IPUN2B

0 = No effect

1 = Punch group kerma factors by reaction and total (for MLINK2 $\neq$ 2 only total is available)

2 = Write group kerma factors on tape by reaction type and total (for MLINK2 $\neq$ 2 only total is available)

3 = Both 1 and 2

CARD NO. 8	FØRMAT (12I6)
KEY	1 = Process all reactions on ENDF/B tape for that material
	2 = Process only the reactions specified as input in array IREACT (specified on Card No. 17, MLINK2 must be 2)
IWXS	Weighting option for the multigroup cross sections.
	1 = Flat weighting
	2 = 1/E weighting
	3 = Weighting function is input
	4 = Weighting function is the input function multiplied by 1/E
	5 = $1/\sigma_t$ weighting
	6 = $1/(E\sigma_t)$ weighting
IWKF	Weighting option for group kerma factors.
	Options 1, 2, 3, 4, 5, and 6 are the same as for IWXS.
INEP	1 = Calculate energy points for pointwise energy mesh
	2 = Read energy points for pointwise energy mesh
NRANGE	Number of energy ranges with equal lethargy interval ($\leq$10) (used only with INEP = 1).
IGAM	Neutron energy group structure option.
	1 = GAM-II 100-group structure
	2 = Input the energy group structure
	3 = Group structure is that of the CTR-library (171 neutron groups)
NØFIS	1 = Process fission
	2 = Do not process fission (for fissionable materials MLINK2 must be 2)
IGAMMA	0 = No effect
	1 = Generate the multigroup gamma production cross sections
MLINK2	1 = Neutron kerma factor calculations via the direct gamma production path (gamma-ray energies calculated from ENDF/B gamma production files)
	2 = Neutron kerma factor calculations via the indirect gamma production path (using neutronics content, files 1-5, only)
	3 = Same as 1 but modified neutron kerma factors are calculated that have the gamma energy added to the local energy release

NNGEXS	Gamma energy group structure option 0 = No effect 1 = Group structure is the built-in 21 groups 2 = Group structure is the built-in 36 groups 3 = Input the energy group structure
NGEXS	Number of gamma energy groups ($\leq$100)
NDEC	Number of cards used for decay energies

CARD NO. 9 FØRMAT (2I6, E12.4)

This card is entered only if NØFIS = 1 and provides instructions for calculating neutron kerma factors from the fission reactions.

KFIS1	1 = Q-value for fission is from ENDF/B data 2 = Q-value for fission is input (as QFIS below) 3 = Energy deposition per fission reaction is input (as TAB1 record specified later)
KFIS2	0 = No effect 1 = Subtract νE_n from the Q-value (used with KFIS1 = 1 or 2)
QFIS	Q-value for fission

CARD NO. 10 FØRMAT (9I6)

This data card provides specifications for the "MACK-Activity-Table" and is entered only if LINK1B $\neq$ 0 and/or, LINK2B $\neq$ 0 and/or IGAMMA $\neq$ 0.

NØACT	0 = No effect 1 = Prepare activity table
IØACT	Logical unit for output requested by IPUN5 (the default value is 19)
IHM	Activity table length
NØKGAM	0 = No effect 1 = Gamma kerma factors are input to be included in the activity table
NØDPA	0 = No effect 1 = Atomic displacement cross sections are input to be included in the activity table 2 = Two sets of atomic displacement cross sections are input to be included in the activity table

MAXPØS	Maximum number of positions to be filled with data in the activity table (positions MAXPØS+1 to IHM are filled with zero; default value for MAXPØS is IHM)
IPRT5	0 = No effect 1 = Print activity table
IPUN5	0 = No effect 1 = Activity table is written in FIDØ card image format on logical unit IØACT
IØGAM	0 = No effect 1 = Write gamma production cross sections on tape

CARD(s) NO. 11 FØRMAT (12I6)

This card(s) is entered only if INEP = 1.

NIR(1)	Number of energy points in Range No. 1 (see detailed input data notes)
NIR(2)	Number of energy points in range No. 2
.	.
.	.
.	.
NIR(NRANGE)	Number of energy points in the last range. NOTE: The user must ensure that NEP = 1 + $\sum_i$NIR$_i$.

CARD(s) NO. 12 FØRMAT (6E12.4)

This may be one or two cards and is entered only if INEP = 1

ERB(1)	Lowest energy for range No. 1 (= lowest point for the energy mesh)
ERB(2)	Lowest energy for range No. 2 (= highest energy ion range No. 1)
ERB(3)	Lowest energy for range No. 3
.	.
.	.
.	.
ERB(NRANGE)	Lowest energy for range number NRANGE
ERB(NRANGE+1)	Highest energy for range number NRANGE (= highest energy point for the energy mesh)

CARD(s) NO. 13 FØRMAT (6E12.4)

This set of cards is required only if INEP = 2.

EP(1)	Energy point No. 1 (lowest energy)
EP(2)	Energy point No. 2
.	.
.	.
.	.
EP(NEP)	Energy point number NEP (highest-energy)

CARD(s) NO. 14 FØRMAT (6E12.4)

This set of cards is required only if IGAM = 2 and one (or all) of LINK1B, LINK2B, and IGAMMA is nonzero. It consists of the desired neutron energy group structure.

EGRPB(1)	Neutron energy group boundary No. 1 (lowest energy)
EGRPB(2)	Neutron energy group boundary No. 2
.	.
.	.
.	.
EGRPB(NGRPS)	Neutron energy group boundary number NGRPS
EGRPB(NGRPS+1)	Neutron energy group boundary number NGRPS+1 (highest energy)

CARD(s) NO. 15 FØRMAT (6E12.4)

This set of cards is entered only if NNGEXS = 3. It consists of the gamma energy group boundaries. There are NGEXS+1 entries.

GEXS(1)	Gamma energy group boundary No. 1 (lowest energy)
GEXS(2)	Gamma energy group boundary No. 2
.	.
.	.
.	.
GEXS(NGEXS)	Gamma energy group boundary NGEXS
GEXS (NGESX+1)	Gamma energy group boundary NGEXS+1 (highest energy)

CARD NO. 16 FØRMAT (E12.4, 4A4)

CØNVF	Conversion factor to convert neutron kerma factors from electron volt-barn/atom to any desired units
UNTHØL	Maximum of 16 alphanumeric characters describing the units of neutron kerma factors after CØNVF is used

CARD(s) NO. 17 FØRMAT (12I6)

This can be one or more cards and is entered only if KEY = 2 and consists of the number of reactions and the MT number for each reaction desired.

NREACT	Number of reactions to be processed for this material
IREACT(1)	MT number for the first reaction to be processed
IREACT(2)	MT number for the second reaction to be processed
.	.
.	.
.	.
IREACT(NREACT)	MT number for the last reaction to be processed

CARD(s) NO. 18 FØRMAT (3(I12,E12.4))

This card set is entered only if NDEC is greater than zero. The decay energies for the various reactions are entered in units of electron volts identified by MT numbers.

MTED(1)	MT number for the first decay reaction
EDEC(1)	Average decay energy for the reaction MT = MTED(1)
MTED(2)	MT number for the second decay reaction
EDEC(2)	Average decay energy for reaction MT = MTED(2)
.	.
.	.
.	.

CARD(s) No. 19

This set of cards is required if IWKF = 3 or 4 or IWSX = 3 or 4 and it consists of the weighting function plus the interpolation scheme. The format of the card set is a standard ENDF/B TAB 1 record (except for N1 and N2 on the first card). The weighting function must be tabulated from low to high energy.

CARD NO. 19.1 FØRMAT (2I11)

Name	Description
N1	Number of interpolation ranges
N2	Number of weighting function points

CARD(s) NO. 19.2	FØRMAT (6I11)
Name	Description
NBT(1)	Last point number in first interpolation range.
JNT(1)	Interpolation scheme for first range
NBT(2)	Last point number in second interpolation range
JNT(2)	Interpolation scheme for second range
.	.
.	.
.	.
NBT(N1)	Last point number in the N1 interpolation range
JNT(N1)	Interpolation scheme for the N1 range
CARD(s) NO. 19.2	FØRMAT (6E12.4)
X(1)	First energy point ($\leq$ lowest energy)
Y(1)	Weight at this energy
.	.
.	.
.	.
X(N2)	Last energy point ($\geq$ highest energy)
Y(N2)	Weight at this energy

CARD(s) NO. 20

This set of cards is required only if NØFIS = 1 and KFIS1 = 3 and it consists of the energy deposition per fission reaction and is similar in format to Card Set No. 19.

Card No. 20.1	FØRMAT (2I11)
Name	Description
N1	Number of interpolation ranges
N2	Number of energy points
Card No. 20.2	FØRMAT (6I11)
NBT(1)	Lost point number in the first interpolation scheme
JNT(1)	Interpolation scheme for first range
.	.
.	.
.	.

NBT(N1)	Last point number in the N1 interpolation range
JNT(N1)	Interpolation scheme for the N1 range

Card(s) No. 20.3 FØRMAT (6E12.4)

X(1)	First energy point (lowest energy)
Y(1)	Energy deposition for fission at this energy
.	.
.	.
.	.
X(N2)	Last energy point (highest energy)
Y(N2)	Energy deposition for fission at this energy

CARD(s) NO. 21 FØRMAT (6E12.4)

This data set is required only if NØACT = 1 and NØKGAM = 1. It contains the gamma kerma factors in NGEXS gamma group structure to be included in the activity table.

XG(1)	The gamma kerma factor for the first group (the highest energy group)
XG(2)	The gamma kerma factor for the second gamma group
XG(NGEXS)	The gamma kerma factor for the NGEXS gamma group (the lowest energy group)

CARD(s) NO. 22 FØRMAT (6E12.4)

This data set is required only if NØACT = 1 and NØDPA = 1 or 2. It contains one set of atomic displacement cross sections in NGRPS neutron group structure to be included in the activity table.

DPA(1)	The atomic displacement cross section for the first neutron group (the highest energy group)
DPA(2)	The atomic displadement cross section for the second neutron group
.	.
.	.
.	.
DPA(NGRPS)	The atomic displacement cross section for the NGRPS neutron group (the lowest energy group)

CARD(s) NO. 23 FØRMAT (6E12.4)

This data set is required only if NØDPA = 2. It contains the second set of the atomic displacement cross sections. The format is identical to that of Card(s) No. 22.

NOTE:

Cards 1 and 2 are read in the MAIN program. Cards 19 and 20 are read in Subroutine IN5. Cards 19 and 20 are read in Subroutine WEITF. Cards 21, 22, and 23 are read in Subroutine ACT.

B. Detailed Input Data Notes

A detailed definition of selected parameters of input data is presented next.

CARD NO. 2

NDFB can vary from one material to another in a single run.

An incorrect IDTAP will result in an error message but will not hinder the execution. Selection of IREW = 1 for a material causes a rewind of the ENDF/B tape on logical unit NDFB prior to searching the tape for the material. By effective use of NDFB and IREW parameters, materials can be processed from several tapes in any order desired. It should be remembered, however, that a rewind operation on a large number of records is expensive.

Parameter IRESØN is a flag for resonance calculations. If the resonance parameters are present in ENDF/B file 2 for a material, the resonance cross sections must be calculated for elastic scattering, radiative capture, fission and total and added to the appropriate data in file 3.

In general, IRESØN = 1 is used and the MACK code will perform the resonance calculations if resonance parameters are found in file 2 of ENDF/B. The options IRESØN = 0 or 2 are provided for special applications.

IRESØN = 0 hinders the execution of the resonance calculations. Since the resonance calculations are generally computer-time consuming, this option should be used if the resonance calculations are not required for the problem being executed. This can occur, for example, if the energy range for the problem is above the resonance energy range; or if elastic scattering, radiative capture, and fission are not among the reactions selected.

If IRESØN = 2, the code will skip the detailed resonance calculations and expects the resonance cross sections on an input tape (logical unit IØ17). The tape may be the output saved from a previous MACK run for the same material or produced by any other means (e.g. from the AMPX or MC^2 code systems). Instructions for the format of this tape are given below.

CARD NO. 6

If IRESØN = 2, the MACK code expects a resonance cross section tape on logical unit IØ17. The cross sections must include both the resonance contribution plus the background and should be Doppler-broadened if desired. In other words, the cross section for each of the resonance reactions (elastic, radiative capture, fission, and also the total) must be the "all" cross section (i.e. the equivalent of the sum of file 2 and file 3 contributions). The energy mesh at which the cross sections are given is arbitrary and can vary from one reaction to the other; but it must be fine enough to permit accurate representation of the cross sections in the resonance region.

MACK-IV calculates the pointwise cross sections for the total, elastic, fission, and radiative capture over the pointwise (kerma) energy mesh (EP) from the data on the input tape (logical unit 17). These calculations are divided into two regions: The first is the resonance energy range whose lower and upper boundaries are specified by the parameters ELØR and EHIR on CARD NO. 6. In this resonance energy range, the cross sections for each point of the EP mesh in this range are obtained by averaging. This averaging is very important as the energy mesh EP is generally not fine enough to accurately represent the point values of the cross sections in the resonance region. In the second energy range (i.e. EP(I) < ELØR or EP(I) > EHIR, the cross sections are obtained by interpolation.

The number of reactions for which cross sections are given on the resonance cross section tape is specified by the parameter NRST on CARD NO. 6. Normally, NRST = 3 in the absence of fission and NRST = 4 for fissionable materials. Cross sections must be arranged on the tape in the order of increasing MT number, i.e. total (MT = 1), elastic (MT = 2), fission (MT = 18), and radiative capture (MT = 102). Reactions not required for calculations in the rest of the problem do not need to be included but their inclusion on the tape is permissible. If the cross sections for a requested reaction are not available (or out of order on the tape) the code will print an error message and terminates the problem.

For each resonance reaction, MACK-IV expects (reads) three unformatted records.

READ(17)MAT, MF, MT, ZA, AWR, IZ, LFS, IZ, IZ

READ(17)MAT, MF, MT, T, Q, IZ, IZ, N1, N2, (NBT(N),JNT(N),N=1,N1),
(X(N),Y(N),N=1,N2)

READ(17)MAT, MF, IZ, FZ, FZ, IZ, IZ, IZ, IZ

The variables MAT, MF, MT, ZA, AWR, and LFS are similar to the ENDF/B notation. The file number MF should be written as 3. Q is the potential scattering cross section. The values of IZ and FZ should be 0 and 0.0. T is the temperature used for Doppler broadening. N1, N2, NBT, JNT, X, and Y represent a TAB1 record for the cross sections. The energy mesh X can be selected by the user and can vary from one reaction to another as discussed above.

The only information actually used by the code are the MT number and the TAB1 record. Other variables are merely printed out or used as internal flags.

The parameters MAXN1 and MAXN2 on CARD NO. 6 correspond to N1 and N2, respectively. MAXN1 must be equal to or greater than the largest N1 used for any reaction on the resonance tape. Similarly, MAXN2 must be greater than the largest N2. MAXN1 and MAXN2 are used internally by MACK to determine the size of the arrays required to read in the cross sections from the resonance tape.

CARD NO. 7

This card provides the options for the various types of calculations and the modes of output. Notice the conditions stated for this card. For example, if LINK2A is selected equal to 1, then LINK1A must be 1. As shown clearly in the flow chart in Fig. 1, the pointwise cross sections must be processed if kerma factors are to be calculated.

CARD NO. 8

KEY = 1 is the normal mode. By selecting KEY = 2 the user can select only specific reactions (specified on CARD NO. 17) for processing.

IWXS and IWKF are the weighting option for multigroup cross sections and multigroup kerma factors, respectively. IWXS or IWKF = 5 or 6 require that the total cross section be available on the ENDF/B tape; if the total cross section is not present the code changes IWXS and IWKF from 5 to 1 or from 6 to 2.

Parameters INEP and NRANGE are discussed in connection with CARDS 11-13. The parameter NØFIS controls processing of the fission reaction. While fission

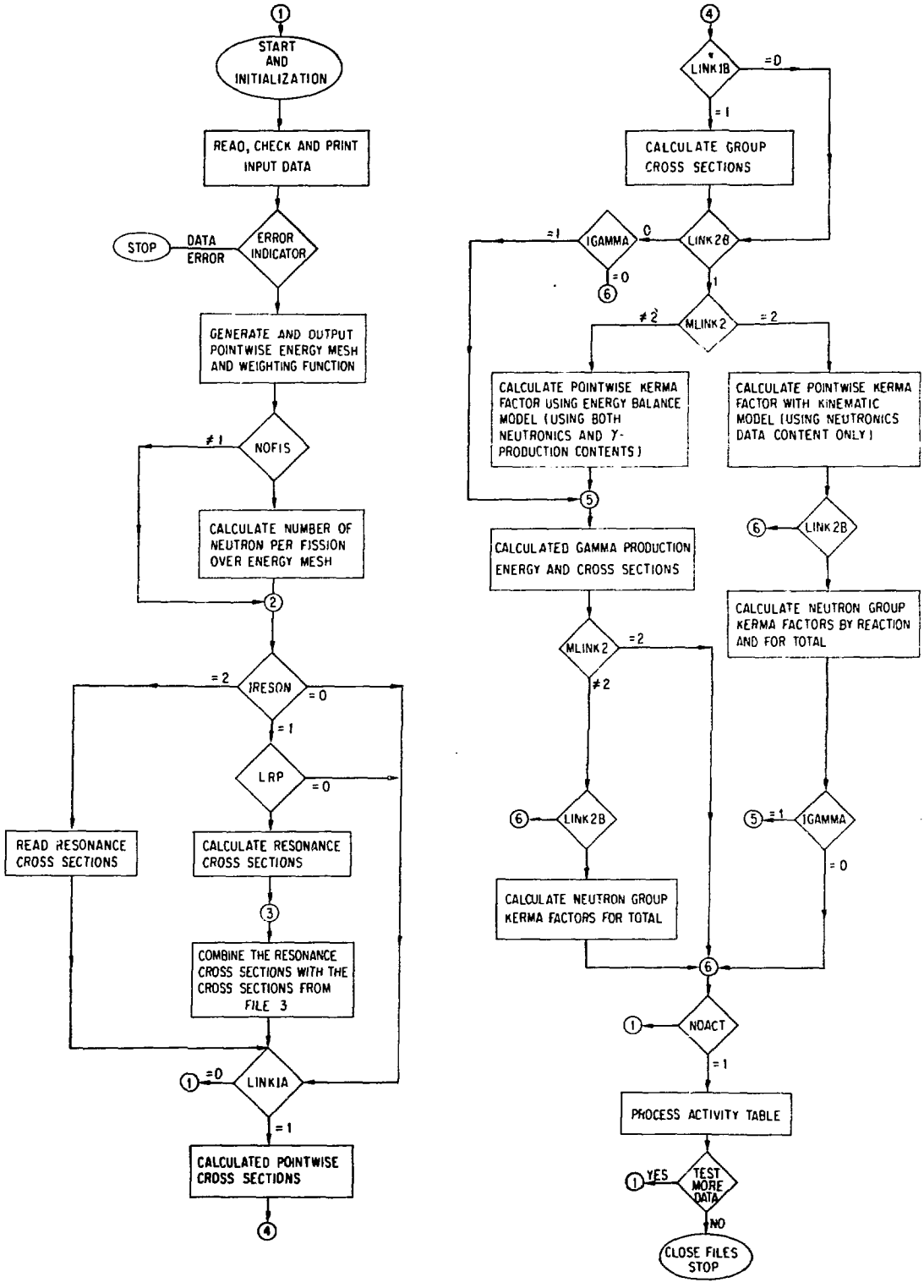


Fig. 1. A flow diagram for MACK-IV.

can be excluded by using KEY = 2 and entering reactions on CARD NO. 17 that do not include fission, the NØFIS parameter is provided for convenience in including or excluding fission by using KEY = 1 and NØFIS = 1 or 2.

If IGAMMA = 1, then NNGEXS must be nonzero.

MLINK2 defines the methodology for calculating the neutron kerma factors. The direct gamma-production path (MLINK2 = 1) and the indirect gamma path (MLINK2 = 2) were discussed in the previous section on calculational algorithms. MLINK2 = 3 provides for calculating "pseudo-kerma factors" that are not truly neutron kerma factors. The true neutron kerma factor for a reaction is the product of the reaction cross section and E_{Hi} the energy deposited within a negligible site of collision as defined in Eq. (9) in the previous section. The pseudo-kerma factor is the product of the reaction cross section and $(E_{Hi} + E_{\gamma i})$ where $E_{\gamma i}$ is the energy carried away with the gamma rays emitted in the reaction. The energy integral of the product of the neutron flux and the pseudo kerma factors gives the total nuclear heating assuming the secondary gamma rays are deposited at the site of the neutron collision. Obviously, this is an approximation that should not be used except in special applications.

Information about the gamma-group structure (NNGEXS and NGEXS on CARD NO. 8 and the energy-group boundaries on CARD NO. 15) is required only if the gamma-production cross sections are requested (IGAMMA = 1) or the gamma-kerma factors are to be included in the MACK-Activity-Table (NØKGAM = 1 in CARD NO. 10).

Notice that if MLINK2 = 1 (kerma factors calculated by the direct gamma-production path) and the gamma-production files for the material are not found on the ENDF/B tape, MACK will change MLINK2 to 2 (indirect gamma-production path). If this occurs the code prints a message to this effect.

CARD NO. 9

The kerma factor for fission at energy point is given by

$$k_f = \sigma_f E_{Hf} ,$$

where σ_f is the fission cross section and E_{Hf} is the energy deposition per fission reaction. If KFIS1 = 1 or 2 on CARD NO. 9, E_{Hf} is calculated as

$$E_{Hf} = Q_f + E_{df} - J(\nu E_n),$$

where Q_f is the effective Q-value for fission. Q_f is taken as the Q-value for MT = 18 in ENDF/B if KFIS1 = 1 or equal to QFIS entered on CARD NO. 9 if KFIS1 = 2. The parameter J is equal to KFIS2 (=0 or 1) entered on CARD NO. 9. The quantity νE_n is the total kinetic energy of all neutrons emitted in the fission process. E_{df} is the value of the decay energy for fission and is taken equal to the decay energy entered on CARD NO. 18 for MT = 18. The prompt gamma energy is subtracted from Q_f if MLINK2 = 1.

If KFIS1 = 3, E_{Hf} is calculated as follows:

$$E_{Hf} = F + E_{df},$$

where F is the kinetic energy of the fission fragments entered on CARD NO. 20.

CARD NO. 10

The first eight parameters on this card define the options for generating the MACK-Activity-Table. These tables are extremely useful for use directly with transport codes to obtain the rates of nuclear heating, tritium breeding ratio, dpa, helium and hydrogen production, and other reaction rates of interest. If NØACT = 1, these tables are prepared by MACK-IV and outputted on logical unit IØACT. The part of the code that generates the activity table arranges the previously processed multigroup cross section, and multigroup kerma factors as well as the multigroup response functions that are entered on CARDS NOS. 21-23.

The number of activity tables is IGM = NGRPS + NGEXS where NGRPS (input on CARD NO. 2) is the number of neutron energy groups and NGEXS (input on CARD NO. 8) is the number of gamma energy groups. Thus, if NGEXS is greater than zero, activity tables in the form of coupled neutron-gamma data can be easily obtained for use with transport calculations that employ coupled neutron-gamma cross sections. The length of the activity table for each group is IHM. The number of entries that are filled with actual data is MAXPØS; the rest of the entries MAXPØS + 1 through IHM are filled with zero. Obviously MAXPØS must be less than or equal to IHM.

If the number of gamma groups, NGEXS is greater than zero, the gamma kerma factors can be read in on CARD NO. 21 provided that NØKGAM = 1 on CARD NO. 10. MACK-IV does not calculate the atomic displacement cross sections at present. However, these cross sections can be inputted on CARD(s) NO. 22 if NØDPA = 1. A provision has been made for inputting a second set of displacement cross sections (or damage function) on CARD(s) NO. 23 if NØDPA = 2.

The position and type of each response function in the MACK-Activity-Table is shown in Table III. The first 34 (or MAXPØS if MAXPØS < 34) positions are fixed; for example, the neutron kerma factor is always in position 1 and the tritium-production cross section is in position 7. Positions 35 through IHM are filled with multigroup reaction cross sections for reactions available in ENDF/B in the order of increasing MT number provided the reaction does not have a reserved position (i.e. if it is not already included in positions 1-34).

Tables for groups 1 through NGRPS contain the response functions for neutron interaction while the tables for groups NGRPS+1 through IGM (where IGM = NGRPS+NGEXS) contain the response functions for gamma interaction. Thus, in reference to Table III, it follows that position 3, which is reserved for gamma-kerma factor is always zero in the tables for groups 1 through NGRPS. One can also note that for groups NGRPS+1 through IGM only positions 1, 3, 32, and 34 have nonzero entries. For position 1, the neutron kerma factors appear in groups 1 through NGRPS and the gamma-kerma factors appear in groups NGRPS+1 through IGM. Similar observations can be made about position 32.

The MACK-Activity Table can be used with any neutron and gamma-ray flux spectra to calculate the spatial distribution of neutron-, gamma-, and total heating, rates of atomic displacements, tritium-breeding ratio, gas production, and other reactions of interest. Since the response functions in the MACK-Activity-Table are flux- and density-independent, the library can be utilized for calculating the nuclear responses in one-, two-, and three-dimensional geometries for any spatial distribution of mixtures of materials.

One way to calculate the nuclear responses is to employ a simple computer program to carry out the summation over energy groups of the product of the flux and the appropriate response function from the MACK-Activity-Table. Another way is to mix the activity tables explicitly with the "regular transport" multigroup cross sections via the mixing tables in the transport code employed to predict the flux solution (e.g., via the 10$, 11$, and 12* arrays in ANISN or the

equivalent in DØT). The number density for each activity table should be the appropriate number for the material multiplied by a small (e.g. 10-]5) fixed number, f. This multiplication factor ensures that the transport cross sections are not significantly altered. The reaction rates and other integrated responses calculated directly by the transport codes will be the true values multiplied by f. For this procedure to be successful the group structure of the multigroup transport cross sections must be identical to that of the MACK-Activity-Tables and the length of the cross section table (IHM) must be the same. In most applications, IHM = IGM + 3.

The reactions included in calculating helium, hydrogen, and tritium-production cross sections are shown in Table IV.

CARDS NOS. 11-13

This set of cards flexibly specifies the pointwise energy mesh for which the pointwise cross sections and pointwise kerma factors are generated. Since the multigroup reaction cross sections and multigroup kerma factors are generated from the pointwise data, the pointwise energy mesh must be chosen with great care. All energies in the input are entered in units of electron volts and in order of increasing energy. The number of energy points is NEP and is entered on Card No. 2. The parameter INEP entered on CARD NO. 8 specifies the option for generating the pointwise energy mesh.

If INEP = 2, CARDS NOS. 11 and 12 should not be entered and the energy mesh is entered on the next card (CARD NO. 13) in the order of increasing energy. The number of entries must be equal to NEP.

The energy mesh is generated by the code at NEP points if INEP is specified as 1. CARDS NOS. 11 and 12 are needed in this case and they specify the characteristics of the energy mesh. The total energy range is divided into a number of energy ranges given by the parameter NRANGE specified on CARD NO. 8. The energy breakpoints for these ranges are entered in the array ERB which has NRANGE + 1 entries. Each range, i, is divided into a number of intervals, NIR_i, of equal lethargy width. The energies of the boundaries for these intervals define the points for the energy mesh. Figure 2 shows how the energy mesh is constructed from the input parameters.

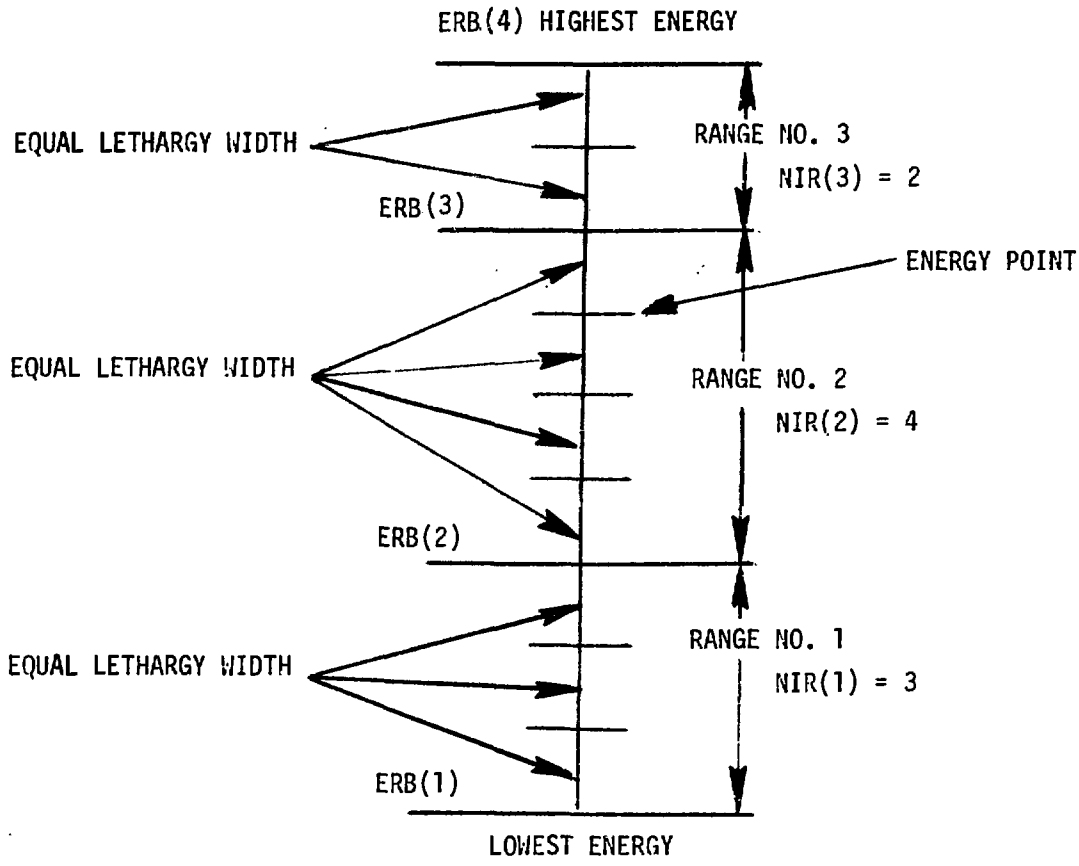
TABLE IV

Reactions Included (MT Nos.) in Calculated Helium, Hydrogen, and Tritium Production

Helium		Hydrogen		Tritium	
MT	m[a]	MT	m	MT	m
22	1	28	1	33	1
23	3	32	1	36	1
24	1	33	1	(51-91)[b]	b
25	1	35		105	1
29	2	36	1	113	1
30	2	(51-91)[b]	1		
34	1	103	b		
35	2	104	1		
36	2	105	1		
(51-91)[b]	b	111			
106	1	112	1		
107	1	113	2		
108	2	114	1		
109	3		1		
112	1		1		
113	2				
114	2				

[a]Multiplicity (No. of particles emitted)

[b]Each reaction of MT = 51-91 with an LR flag is treated as a reaction with an MT equal to LR.



EP(1) = ERB(1) (lowest energy)

EP(NEP) = ERB(4) (highest energy)

NRANGE = No. of energy ranges = 3

NEP = No. of energy points in the mesh

$$= 1 + \sum_{i} NIR_i$$

$$= 10$$

Fig. 2. Schematic diagram showing an example for the relation between the energy mesh parameters

CARD NO. 14

This set of cards defines the neutron energy group structure if none of the built-in group structures is adequate. The number of entries is NGRPS + 1. The energy group breakpoints are entered in order of increasing energy. The energy group limits must be within the limits of the energy point mesh if group kerma factors are desired. Group kerma factors for a group (or portion of a group) outside the limits of the energy point mesh are set to zero. Group cross sections are calculated directly from ENDF/B data and will be calculated correctly regardless of the energy range of the point energy mesh, provided that the range of ENDF/B data covers the energy limits of the group structure. ENDF/B data usually covers the energy range from 10^{-5} eV (or the reaction threshold energy) to 30 MeV.

CARD NO. 15

This set of cards defines the gamma-group structure if NNGEXS = 3. The number of entries is NGEXS + 1. The energy breakpoints are entered in the order of increasing energy.

CARD NO. 16

MACK calculates the energy release per reaction in units of electron volts and the cross sections are in units of barns per atom; hence, the calculated kerma factors (microscopic) are in units of electron volt-barn/atom. The conversion factor, CØNVF, entered on CARD NO. 16, is used by the code to convert the kerma factors into any other desired units. CØNVF can also be used to obtain the macroscopic kerma factors for the material by including the nuclide density x 10^{-24} in it. CØNVF should be entered as 1.0 if no conversion is desired; and in this case UNTHØL should be entered as EV.BARN/ATOM or any equivalent character.

CARD NO. 17

If KEY = 2 (on CARD NO. 8) only selected reactions will be processed according to the input on CARD(s) NO. 17. NREACT defines the number of reactions to be processed. The MT numbers for the desired reactions are entered in any desired order. The MT numbers for all reactions are those defined by the ENDF/B manual (see Appendix B). If any of the MT numbers 103-107 [(n,p), (n,d),

(n,t), (n,^{3}He), (n,α)] are specified, the corresponding reactions in the 700's series [reaction cross sections to various levels, e.g. (n,p_0), (n,p_1), etc.] are also processed.

CARD NO. 18

The number of cards entered here is equal to NDEC as specified on CARD NO. 8. If NDEC = 0, no cards should be entered. The cecay energies for the various reactions are entered on these cards in units of electron volts.

Each reaction for which a decay energy is entered requires two fields (each field is 12 columns). The reaction MT number (same MT as that of ENDF/B, see Appendix B) is entered in a field and the decay energy of the reaction is entered in the second field. Pairs of a reaction number and decay energy can be entered in any order of MT (for example, they need not be in an increasing order of MT). Decay energies for the MT-700's series can also be entered. If an MT number is entered which is not defined in ENDF/B the decay energy for this reaction is ignored.

A default value of zero is used for the decay energy of any reaction which is not entered on this set of cards.

CARD(s) NO. 19

The format of this card is similar to an ENDF/B TAB 1 record. The following brief explanation of the card set is intended for users not familiar with ENDF format.

The weighting function is entered as tabulated points in pair of X and Y(X). The number of pairs is N2. The X array is the energy points and Y has the values of the corresponding weighting function. The pairs are ordered by increasing values of X.

The interpolation scheme defined on CARD NO. 19.2 is used for interpolation between input values. The energy range is broken into N1 ranges. JNT(I) is the interpolation scheme identification number used in the I-th range. NBT(I) is the point number separating the I-th and the (I + 1)-th interpolation ranges.

The allowed interpolation schemes are:

JNT	Description
1	y is constant in x
2	y is linear in x
3	y is linear in ln x
4	ln y is linear in x
5	ln y is linear in ln x

It should be obvious that NBT(N1) = N2. In case of one interpolation scheme throughout the energy range, one should simply enter

```
N1 = 1
NBT(1) = N2
JNT(1) = I
```

where I is chosen from the above table.

Input/Output Data Sets - Logical Unit Assignments

The logical unit numbers are integer variables. Their numeric values are defined in subroutine START. The data sets required in a run are problem dependent. The type and purpose of these data sets are as follows:

a. Logical Unit 5 is a formatted input data set in a card image form (usually card reader).

b. Logical Unit 6 is a formatted output data set with a record length = 133 characters (usually line printer).

c. Logical Unit 7 is a formatted output data set in a card image form (usually card punch).

d. Logical Unit 8 is a formatted output data set in a card image form. It is required for multigroup neutron reaction cross sections (IPUN1B < 0) or multigroup kerma factors (IPUN2B < 1) outputs.

e. Logical Unit 9 is a formatted output data set in a card image form. It is required for pointwise kerma factor (IPRT2A > 1) outputs.

f. Logical Unit NDFB (default 10) is an ENDF/B library data set. The data set type depends on the value given for the input variable MØDE.

g. Logical Units 11, 12, 13, 14, 15, and 16 are scratch unformated data sets required for resonance calculations. Also, Units 11, 12, 13, and 14 data sets are used as scratch unformatted data sets for gamma calculations. Logical Unit 16 stores the pointwise corss sections by reaction for use by the code during the calculations. Logical Unit IØ17 (dault 17) used as an unformatted input data file if IRESØN = 2. If IRESØN = 1, logical unit IØ17 (default 17) is used to write the resonance cross sections calculated in MACK.

h. Logical Unit 18 is a scratch unformatted data set required for storing $\cos(\theta_{cm})$ (average of the cosine of the center-of-mass scattering range) as a function of incident neutron energy for the different reactions; always required.

i. Logical Unit IØACT (default 19) is a formatted output data set used for activity table output (NØACT = 1).

j. Logical Unit 20 is an unformatted output data set used for gamma production matrix [(IGAMMA = 1 or MLINK2 = 2) and IØGAM = 1].

IV. OUTPUT DESCRIPTION

The MACK program provides the output in several forms, printed, punched, and/or written on tape. The purpose of this section is to present some useful remarks about the various modes of output.

A. Printed Output

The printed output is self-explanatory. The brief description given below is intended to ensure a correct interpretation of the output.

The first output section is an edit of the input data. This includes the input parameters, the energy mesh (read in or generated according to input instructions), and the weighting function. A message is then printed if the ENDF/B tape identification is different from the IDTAP given in the input. The code checks some (but not all) of the input data and if any error is found, self-explanatory messages are printed and the run is terminated.

The following section is a printout of the descriptive section of ENDF/B file 1 of the material and serves as a short documentation of how the data for the material was evaluated. Included in this section is a "dictionary" of the type of data available in the evaluation. For fissionable materials, the number of neutrons, $\nu(E)$, emitted per fission is printed.

For resonance nuclides, the calculation in the resonance processor follow if resonance parameters are available in file 2 and IRESØN = 1 in the input. If JWRIT = 1 the calculated resonance cross sections for total (MT = 1), elastic (MT = 2), fission (MT = 18), and radiative capture (MT = 102) are printed. This is often a bulky output. The cross section printed here is the "all" cross section, i.e. it includes the resonance cross section with Doppler broadening — if any — added to the "background" from file 3. The energy mesh is the fine mesh that is generated internally in the code. If the resonance cross sections are read in (IRESØN = 2), the cross sections printed here are simply an edit of the data read from the input tape. Following this part is the output from "AVGRES". This output consists of the total, elastic, fission and radiative capture "point average" cross sections at the broader pointwise energy mesh specified or read in the input (kerma energy mesh). The "point average" cross sections are obtained from the fine-energy mesh by averaging in the resolved resonance energy range and interpolating in the other energy ranges.

The cross sections by reaction follow. The cross section for each reaction is titled by the ENDF/B MT number and description and LR flag and description of the corresponding reaction (currently, LR has a meaning only for MT = 51-91). A list of ENDF/B reaction numbers, MT, is given in Appendix B. The MT reaction Q-value is also printed. If LR is not zero, both the Q-value for the (n,n') part of the reaction and the Q-value corresponding to the combined reaction LR are printed. For each reaction, the group cross sections are printed (if both LINK1B and IPRT1B are 1) followed by pointwise cross sections (if both LINK1A and IPRT1A are 1). A message is printed in this section about each reaction searched for and not found on the ENDF/B tape.

The next section of the output is the kerma factors if LINK2A = 1. The average of the cosine of the scattering angle and the average kinetic energy of the secondary neutrons are tabulated by energy points for the appropriate reactions. The type of output for kerma factors depends on the calculational method selected by MLINK2.

If the indirect gamma-production path (neutronics contents only) is chosen MLINK2 = 2), the pointwise kerma factors can be printed by reaction. The print for the pointwise kerma factor of a reaction is a tabulation by energy point of the cross section, energy deposition per reaction, and the kerma factor. The pointwise kerma factors by reaction are printed only if IPRT2A is equal to 1 or 3. The next part of the output is always printed and consists of the total pointwise kerma factor and the contribution to the kerma factor from each of the major reaction types discussed in Sec. II. The kerma factors for each of these reaction types is a sum over the kerma factors of the corresponding MT numbers designated in Table II. If both LINK2B and IPRT2B = 1, the next part of the output is a printout of the energy group kerma factors for each of the major reaction types as well as the total. The group kerma factors are not printed for any kerma-reaction type if it is zero for all energy groups.

On the other hand if the kerma factors are processed via the direct gamma-production path (MLINK2 = 1 or 3) or the gamma-production cross sections are requested (IGAMMA = 1) the program processes the gamma-production files prior to the kerma factor calculations and prints the output for the gamma production first. The output from the gamma processor consists of three parts. The first is the energy-group structure for the neutrons and gamma rays. The second is the photon-production cross-section matrix, and the photon-energy-production

matrix. The third is the total gamma-energy production from each neutron group (gamma energy per atom per unit flux). The gamma-production data is followed by a printout of the kerma factors.

If MLINK2 = 1 or 3 kerma factors by reaction are not calculated and, therefore, are not printed. The pointwise kerma factors for the total are given in a summary table as a function of the neutron energy. The summary table also includes other information that the user must make sure to interpret correctly. This information includes the total pointwise gamma-energy production and seven columns of "pseudo"-kerma factors for seven reaction types. The values for these seven components are not the actual kerma factors for the seven reaction types. They represent the kerma factors plus the gamma energy production. This is different from the output given by the code in the case of MLINK2 = 2 where the actual kerma factors are given by reaction type.

Following the tabulation of the total kerma factor by energy group is a printout of the MACK-Activity-Table if both NØACT and IPRT5 = 1. The activity tables are intended for use directly within the transport codes as described in the detailed input section. The first 34 positions in this table are fixed for the response functions shown in Table III. Positions 35 through IHM are filled with information according to the input instructions. The printout of the activity table is followed by a directory for this table. This directory lists the name of the response function in each position. For reaction cross sections the Q-values are also given in the directory.

The units used in the input data, internally in the code and output (print, punch, and tape) are always in the same set of units used in ENDF, namely

Parameter	Units
Energies	Electron volts
Angles	Dimensionless cosines of the angle
Cross sections	barns
Temperature	degrees Kelvin (°K)
Mass	In units of the neutron mass
Angular distributions	Probability per unit cosine
Energy distributions	Probability per electron volt

except for the final pointwise and energy-group kerma factors which are

converted to units of UNTHØL using the conversion factor CØNVF specified on input data CARD NO. 16.

B. Punched Output

The code generates punched cards for the main output quantities if the appropriate punch options are chosen. The pointwise energy mesh is punched first if the pointwise cross sections or printwise kerma factors are punched. The pointwise quantities are given in increasing order of energy while the group quantities are given in decreasing order of energy. The code punches one card per material as a title card for the punched output. The format for this title card is (18A4, 4HMAT =, I4). The first 18 words are the input title followed by ENDF/B material number. This card serves as a separator between the punched output for the various materials processed in a single run.

The punched output for each section is described below:

Pointwise Cross Sections [IPUN1A > 0]

1. Title Card (CARD NO. 1 in the input data)
2. Reaction Title Card
3. The pointwise cross sections in the order of increasing energy (NEP values per reaction).

Group Cross Sections [IPUN1B > 0]

1. Title Card (CARD NO. 1 in the input data)
2. Reaction Title Card
3. A card with 54* in the first three columns.
4. The group cross sections in the order of decreasing energy (NGRPS values per reaction)
5. A card with T in the third column.

Pointwise Kerma Factors [IPUN2A > 0]

1. Title Card (CARD NO. 1 in the input data)
2. Kerma factor title card

3. The pointwise kerma factor in the order of increasing energy (NEP) values per reaction).

Group Kerma Factors [IPUN2B = 1 or 3]

1. Title Card (CARD NO. 1 in the input data)
2. Kerma factor title card
3. A card with 54* in the first three columns
4. The group kerma factors in the order of decreasing energy (NGRPS values)
5. A card with T in the third column.

The title card in each section has a letter "G" or "P" in column 73. This letter serves as an identifier for the following section until the next title. The letters "P" and "G" indicate pointwise or groupwise information. The format of the reaction card and the kerma factors title card are as follows:

Pointwise Cross Sections	'Point$_\nabla$X-SEC.MT =', I4, '(', 5A4,')', '$_\nabla$LR =', I4, '(', 5A4, ')'
Group Cross Sections	'GROUP$_\nabla$X-SEC.MT =', I4, '(, 5A4,')', '$_\nabla$LR =', I4, '(', 5A4,')'
Pointwise Kerma Factors	'Point$_\nabla$KERMA$_\nabla$MT =', I4, '(', 5A4, ')'
Group Kerma Factors	'GRØUP$_\nabla$KERMA$_\nabla$MT =', I4, '(', 5A4, ')'

The kerma factors reaction numbers were chosen according to ENDF/B specifictions (see Appendix B) of adding 300 to the corresponding reaction. For example, for elastic scattering (MT = 2), the reaction number for the kerma factor for elastic scattering is 302.

C. Output on Logical Unit 8

This is a formatted output data set in a card image form and contains the multigroup reaction cross sections (IPUN1B < 0) or/and the multigroup kerma factors (IPUN2B > 1). This data set is written in the same format as the punched output explained above. The data set is not rewound after each material. Therefore, the output for different materials in a single run can be

written on one data set. An "END-OF-FILE" mark is written on the data set only at the end of the run after all the materials hafe been completed.

D. Output or Logical Unit 9

This formatted output data set is in a card image form and contains the pointwise kerma factors (IPRT2A > 1). This data set is written in the same format as the punched output explained above. If several materials are processed in a single run, the pointwise kerma factors for all the materials are written onto one data set as discussed above for logical unit 8.

E. Output on Logical Unit IØACT (Default = 19)

The MACK-activity tables are written on the logical unit assigned by the input variable IØACT or the default value of 19. This formatted data set is in a card image form. A title card is written followed by the activity table as a two-dimensional array with the entries written in FIDØ format. The number of groups is NGRPS+NGEXS and the number of positions per group is IHM. The data is written in the following order: Group 1, positions 1 through IHM; group 2, positions 1 through IHM; etc. The output for several materials in a single run is written into data set IØACT in the same order they are processed as for logical units 8 and 9 discussed above.

F. Output on Logical Unit 20

This unformatted data set contains the gamma-production cross sections if requested. The first record contains the ENDF/B material number. The second record contains the gamma-production group cross sections in a two-dimensional matrix form with the neutron group index of the matrix running faster than the gamma-group index and from the lower to the higher energy group. The output for several materials in a single run is written on the data set in the same order the materials are processed.

V. MISCELLANEOUS INFORMATION

This section provides the user with additional information about the MACK-IV. The information concerns the operation of the code.

The program utilizes the dynamic storage technique (with only few exceptions) to save on the core storage requirements. Subroutine SIZE has the function of allocating this storage. The subroutine has the following form:

```
SUBRØUTINE SIZE (LIMIT)
CØMMØN/DATA/D(80000)
CØMMØN/CGAMMA/IGAMMA, NNGEXS, NGEXS, IØ11, IØ12, IØ13, IØ14, ICØPY, IRWG,
                      IØGAM, IØ20, IDICL, IDIC(2,500), GEXS(101),
                      STØRE(5000,4)
IDICL = 500
LIMIT = 80000
RETURN
END
```

The size of the array D largely determines the core-storage requirement. The variable LIMIT must be numerically equal to the size of the array D. In general, for materials with no resonance calculations, LIMIT = 60000 is adequate for most uses. If resonance calculations are requested, LIMIT = 80000 is generally sufficient. The calculation of the required core storage as a function of the input parameters is somewhat complex and is carried out in the MAIN program. The code always checks storage requirements versus available storage and prints clear messages. The amount of storage allocated can be adjusted by changing the dimension of the array D (and changing the value of the variable LIMIT accordingly) in subroutine SIZE and recompiling this subroutine.

The other fixed dimensions in CØMMØN/CGAMMA/ that appear in subroutine SIZE above also need explanation. IDICL is the size of the second dimension of array IDIC which is used to store the "Dictionary" of ENDF/B file 1.

GEXS array is used to store the energy group boundaries for the gamma group structure. Its dimension is equal to the number of gamma group plus 1. STØRE is used by GAMMAC subroutine and its dimension is fixed.

The subroutine clock is used to calculate the amount of CPU time used to reach a specified point during the calculations. This subroutine calls a

utility routine 'TLEFT' which is an IBM routine. For a non-IBM user without comparable facilities, a dummy routine should be supplied for "CLOCK' routine as follows:

```
SUBROUTINE CLOCK
RETURN
END
```

Figure 3 shows the overlay structure recommended for the MACK-IV program. This overlay structure is designed to allow one scratch array for the different segments using the dynamic storage technique.

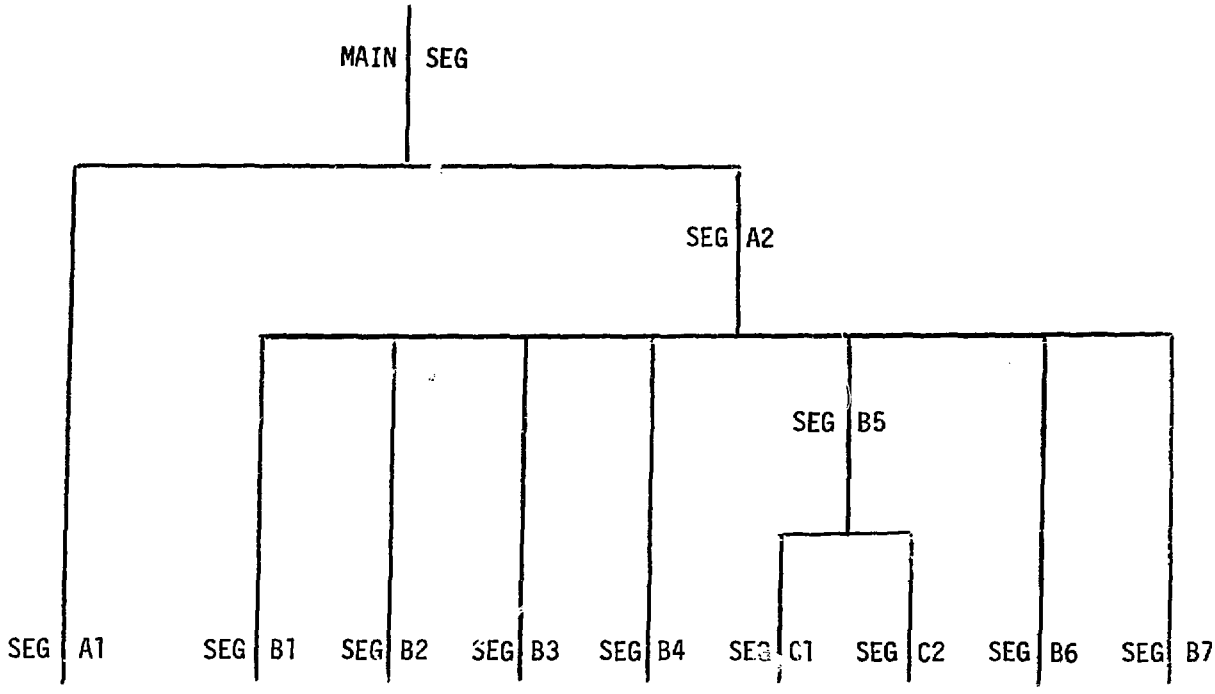


Fig. 3. Overlay structure for MACK-IV

MAIN Segment

MAIN
GRATE
TERP1
CØNT
LIST
TAB1
WT1E
TAB2
WRIT
TPØS
ECSI
SCRAT1
SCRAT
TERPØ
CLØCK

Segment A2

PUNSH
RITE
TERP2
READ3
SAVE
ERRØR
SKPFLL
TRID
TMAT
TMF3
FINDI
MTID
FINDIM
DTFPUN
FLTFX
TITLE

Segment A1

GAMMAC
CØPY
SUB1
LØCT
TERP4
SW

Segment B1

START
SIZE
IN5
EPØINT

Segment B2

WEITF
NUFIS

Segment B3

NPTXS
AVGRES
BRØADN
CØMBR
PMESH
RESP
RRES
URES
WRITES
ASTØR
CAIN
CRØP
FRAN
FUNKY
HUNKY
PHIL
TMF2
URES2
URSSF
VØGAM
FJ
DLAG

Segment C1

EKERMA
INELL
DN2N
TSN2N
RN3N
NPCHG
INELC
GAMMA
CHARG

Segment C2

EKERMB
DN2NB
TSN2NB
NPCHGB
INELLB
INELCB
GAMMAB
CHARGB
RN3NB

Segment B4

XSECN
SIGPR
PUN1B
LØØKMT
READ33
HELIUM
HYDRGN
TRITUM
CRØSG
CØST
TMF4
CMLAB
MUMESH

Segment B5

GETAMU
EBAR
ELAST
FISSN
MATMFS
KERMAG

Segment B6

ACT
OUT6
GETGRP

Segment B7

WEITF
TMF1
HØLL

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APPENDIX A

Sample Problems

Three sample problems are given here for illustration purposes. These sample problems do not cover all the available options in the code. The output from these sample problems is available with the code package. It must be noted that these sample problems do not necessarily represent an actual physical problem.

Sample Problem 1

The neutron kerma factors and the gamma production cross sections are calculated for beryllium MAT No. 1289, from ENDF/B-IV Library. The built-in neutron and gamma group structure is used for this sample. A flat weighting function is used for the multigroup reaction cross sections and the kerma factors. The multigroup reaction cross sections and the multigroup kerma factors are punched on cards. The direct gamma-production path is used for neutron kerma factor calculations.

```
BE      ENDF-IV                                                    OCT 1977
BE          ENDF      1289      10       0       2       1       1  1000   171     17
     0      1      1
     .001           0.9             10.0            300.0
     1      1      1      1       1      1       4      1       0    -2      0       2
     1      1      1      1       3      1       0      1       1     2     21       0
     1     19    210      0       0    210       1      0       0
    19    580    400
      0.00001       1.0         1.0     E06     17.4 E06
  1.0           EV*BARN/ATOM
```

Sample Problem 2

In this sample the multigroup reaction cross sections, the neutron kerma factors, and the gamma-production cross sections are calculated for lithium, MAT No. 1272, from ENDF/B-IV Library. The direct gamma-production path is used for the kerma factor calculations. An input weighting function is used for

neutron cross sections and neutron kerma factors. All the output for the different quantities are saved on the output data sets. The MACK-Activity Table is prepared. A decay energy is given for MT = 28, 102, and 104.

```
 117      ENDF/B-IV                                                    OCT 1977
 LI7          ENDF       1272      10     404       2        1        1  1000     171      17
      0       1          1
      .001                0.9                10.0              300.0
      1       1          1         1        1         1        4        1        0     -2       0        2
      1       3          3         1        3         3        0        1        1      2      36        1
      1      19        210         0        0       210        1        1        1
     19     580        400
      0.00001            1.0              1.0     E06       17.4 E06
   1.0              EV*BARN/ATOM
              28      1.5600E06                 102     9.3100E06              104     1.5600E06
              1             172
           172                2
1.000000-054.834999+009.999996-024.834999+004.139900-011.495000+00
5.315800-012.500000-016.825600-012.500000-018.764200-012.500000-01
1.125400    2.500000-011.445000    2.500000-011.855399    2.500000-01
2.372399    2.458000-013.058999    2.542000-013.927899+002.500000-01
5.0435      2.500000-016.476000    2.500000-018.3153      2.500000-01
1.067700+012.500000-011.371000+012.500000-011.760300+012.499000-01
2.260300+012.500000-012.920299+012.562000-013.726700+012.438000-01
4.785100+012.500000-016.144199+012.500000-017.889299+012.500000-01
1.013000+022.500000-011.300700+022.500000-011.670200+022.500000-01
2.144500+022.500000-012.753599+022.500000-013.535798+022.500000-01
4.540900+022.500000-015.829500+022.500000-017.485198+022.500000-01
9.611199+022.500000-011.234100+032.500000-011.584600+032.500000-01
2.034700+032.500000-012.248700+039.999996-022.485200+039.999996-02
2.612600+034.999000-022.746500+034.998000-023.035400+039.999996-02
3.354600+039.9989950-23.707400+039.999996-024.307398+031.500000-01
5.530797+032.500000-017.101699+032.500000-019.118797+032.500000-01
1.170900+042.500000-011.503400+042.500000-011.930500+042.500000-01
2.187500+041.250000-012.357900+047.500994-022.417600+042.500000-02
2.478800+042.500000-022.605800+044.996000-022.700000+043.551000-02
2.850000+045.407000-023.182800+041.104000-013.430700+047.499999-02
4.086800+041.750000-014.630900+041.250000-015.247500+041.250000-01
5.656200+047.499999-026.737900+041.750000-017.200000+046.632996-02
7.950000+049.908998-028.250000+043.704000-028.651700+044.754000-02
9.803700+041.250000-011.110900+051.250000-011.167900+055.004000-02
1.227700+054.993000-021.290700+055.004000-021.356900+055.002000-02
1.426400+054.995000-021.499600+055.004000-021.576400+054.994000-02
1.657300+055.005000-021.742200+054.996000-021.831600+055.004000-02
1.925500+054.999000-022.024200+054.999000-022.128000+055.001000-02
2.237100+055.000000-022.351800+055.000000-022.472400+055.001000-02
2.732400+059.998995-022.872500+055.000000-022.945200+052.499000-02
2.972000+059.057999-032.985000+054.363999-033.019700+051.156000-02
3.337300+059.999996-023.688300+059.999996-023.877400+055.000000-02
4.076200+055.000000-024.504900+059.999996-024.978700+059.999996-02
5.234000+055.001000-025.502300+054.999000-025.784400+055.000000-02
6.081000+055.000000-026.392800+055.000000-026.720600+055.000000-02
7.065100+054.999000-027.427400+055.001000-027.808200+055.000000-02
```

```
 8.208500+055.101000-028.629400+058.462000-019.071800+058.839999-01
 9.616400+051.080000+001.002600+068.044000-011.108000+062.037000+00
 1.164800+061.075000+001.224600+061.113000+001.287300+061.145000+00
 1.353400+061.181999+001.422700+061.212000+001.495700+061.242999+00
 1.572400+061.270000+001.653000+061.292999+001.737700+061.313999+00
 1.826800+061.332999+001.920500+061.346999+002.019000+061.355000+00
 2.122500+061.356999+002.231300+061.355000+002.306900+069.003000-01
 2.345700+064.493000-012.365300+062.237000-012.385200+062.248999-01
 2.466000+068.900999-012.592400+061.320999+002.725300+061.297999+00
 2.865000+061.270000+003.011900+061.235000+003.166400+061.195000+00
 3.328700+061.150000+003.678800+062.148000+004.065700+061.919000+00
 4.493300+061.667999+004.723700+067.362000-014.965900+066.698999-01
 5.220500+066.050000-015.488100+065.409999-015.769500+064.796000-01
 6.065300+064.206000-016.376300+063.651000-016.592400+062.145000-01
 6.703200+069.899996-027.046900+062.660000-017.408200+062.230000-01
 7.788000+061.844000-018.187300+061.506000-018.607100+061.212000-01
 9.048400+069.607995-029.512300+067.497996-021.000000+075.757000-02
 1.051300+075.003000-021.105200+075.000000-021.161800+074.994000-02
 1.221400+075.003000-021.284000+077.198995-021.349900+077.207999+00
 1.384000+072.453999+011.419100+074.281999+011.455000+073.293999+01
 1.491800+071.096000+011.568300+071.610000+001.648700+075.000000-02
 1.733299+075.004000-02
```

Sample Problem 3

In this problem, carbon is to be processed. The neutron kerma factor is calculated using the indirect gamma model. The weighting function 1/E is used for both of the neutron kerma factors and multigroup reaction cross sections. The neutron group structure is given as input data but the built-in gamma group structure is selected.

```
C12          ENDF      1274      10     408       2        1        1   1000      46      17
      0       1        1
      .001              0.9                10.0                300.0
      1       1        1        1         1        1        4        1        0       3       0       3
      1       2        2        1         3        2        0        1        2       1      21       0
      1       7       49        0         0       49        1        1        0
     19     580      400
      0.00001          1.0              1.0     E06      17.4 E06
     .022000+0        .41399+0         .87642+0         .18554+1         .39279+1         .83153+1
     .17603+2         .37267+2         .78893+2         .16702+3         .35358+3         .74852+3
     .15846+4         .33546+4         .71017+4         .15034+5         .31828+5         .67379+5
     .12277+6         .16573+6         .22371+6         .30197+6         .40762+6         .55023+6
     .74274+6         .10026+7         .13534+7         .18268+7         .24660+7         .27253+7
     .30119+7         .33287+7         .36788+7         .40657+7         .44933+7         .49659+7
     .54881+7         .60653+7         .67032+7         .74082+7         .81873+7         .90484+7
     .10000+8         .11052+8         .12214+8         .13499+8         .14918+8
  1.0          EV*BARN/ATOM
```

APPENDIX B

Definition of Reaction Types in ENDF/B-IV

Reaction types are identified by an integer, MT. The allowed reaction types are listed below. The reaction type number (MT) generally refers to a specific neutron-nucleus interaction mechanism, but occasionally it indicates that a particular type of information is given. The general rules for assignment of MT numbers are:

MT (Range)	Description of Class of Reactions
1-100	Reaction types in which secondary particles of the same type as the incident particles are emitted.
101-150	Reaction types in which no secondary particles of the same type as the incident particles are emitted.
151-200	Resonance region information.
201-450	Quantities derived from the basic data.
451-699	Miscellaneous quantities.
700-799	Excitation cross sections for reactions that emit charged particles.
800-999	(not assigned)

The specific MT assignments are given in the tabulation below. For the most part they are consistent with those used in the UKAEA Nuclear Data File.

MT	Description
1	Total cross section (redundant, equal to the sum of all partial cross sections).
2	Elastic scattering cross section
3	Nonelastic cross section (redundant, equal to the sum of all partial cross sections except elastic scattering).
4	Total inelastic cross section (redundant, equal to the sum of MT = 51, 52, 53, . . ., 90, 91).
5	(to be assigned)

MT	Description
6	(n,2n) cross section for first excited state (describes first neutron).
7	(n,2n) cross section for second excited state (describes first neutron).
8	(n,2n) cross section for third excited state (describes first neutron).
9	(n,2n) cross section for fourth excited state (describes first neutron).
10-15	(to be assigned)
16	Direct (n,2n) cross section [total (n,2n) cross section is sum of MT = 6, 7, 8, 9, and 16].
17	(n,3n) cross section.
18	Total fission cross section (sum of MT = 19, 20, 21, 38).
19	(n,f) cross section (first chance fission).
20	(n,n'f) cross section (second chance fission).
21	(n,2nf) cross section (third chance fission).
22	(n,n'α) cross section.
23	(n,n'3α) cross section.
24	(n,2nα) cross section.
25	(n,3nα) cross section.
26	(n,2n) isomeric state cross section.
27	Absorption cross section (sum of MT = 18 and 101) (includes particle reactions).
28	(n,n'p) cross section.
29	(n,n'2α) cross section.
30	(n,2n2α) cross section.
31	To be used as LR flag only.*
32	(n,n'd) cross section.
33	(n,n't) cross section.

MT	Description
34	(n,n'^{3}He)
35	(n,n'd2α) cross section
36	(n,n't2α) cross section
37	(n,4n) cross section
38	(n,3nf) cross section (fourth chance fission)
39	To be used as LR flag only*
40	To be used as LR flag only*
41-45	(to be assigned)
46	Cross section for describing the second neutron from (n,2n) reaction for first excited state.
47	Cross section for describing the second neutron from (n,2n) reaction for second excited state.
48	Cross section for describing the second neutron from (n,2n) reaction for third excited state.
49	Cross section for describing the second neutron from (n,2n) reaction for fourth excited state.
	(NOTE: MT = 46, 47, 48, and 49 should not be included in the sum for the total (n,2n) cross section.)

*The following MT numbers are used only as LR flags in order to indicate the mode of decay of the residual nucleus:

LR	Description
31	Indicates that gamma emission is the mode of decay of the residual nucleus formed in the primary reaction.
39	Indicates that internal conversion is the mode of decay of the residual nucleus formed in the primary reaction.
40	Indicates that electron-positron pair formation is the mode of decay of the residual nucleus formed in the primary reaction.

(The "primary" reaction could be, for example, an (n,n'), (n,p), (n,α), (n,np), etc., reaction.)

MT	Description
50	(to be assigned)
51	(n,n′) to the first excited state
52	(n,n′) to the second excited state
. . .	
90	(n,n′) to the 40-th excited state
91	(n,n′) to the continuum
92-100	(to be assigned)
101	Neutron disappearance (sum of all cross sections in which a neutron is not in the exit channel) $MT = 101 \text{ is } \sum_{i=2}^{14} (MT - 100 + i)$.
102	(n,γ) radiative capture cross section
103	(n,p) cross section
104	(n,d) cross section
105	(n,t) cross section
106	(n,^{3}He) cross section
107	(n,α) cross section
108	(n,2α) cross section
109	(n,3α) cross section
110	(to be assigned)
111	(n,2p) cross section
112	(n,pα) cross section
113	(n,t2α) cross section
114	(n,d2α)cross section
115-119	(to be assigned)
120	Target destruction = nonelastic less total (n,n′γ)
121-150	(to be assigned)

MT	Description
151	General designation for resonance inforamtion
152-200	(to be assigned for specific resonance information)
201-250	(to be assigned)
251	$\bar{\mu}_L$, the average cosine of the scattering angle (laboratory system for elastic scattering
252	ξ, the average logarithmic energy decrement for elastic scattering.
253	γ, the average of the square of the logarithmic energy decrement for elastic scattering, divided by twice the average logarithmic decrement for elastic scattering
254-300	(to be assigned)
301-450	Energy release rate parameters, $E^*\sigma$, for total and partial cross sections. Subtract 300 from this number to obtain the specifc reaction-type identification. For example, MT = 302 = (300 + 2) denotes elastic scattering.
451	Heading or title information (given only in File 1).
452	$\bar{\nu}$, average total (prompt plus delayed) number of neutrons released per fission event.
453	Radioactive nuclide production
454	Fission product yield data
455	Delayed neutrons from fission
456	Prompt neutrons from fission
457	Radioactive decay data
458-500	(to be assigned)
501	Total photon interaction cross section
502	Photon coherent scattering
503	(to be assigned)
504	Photon incoherent scattering
505-514	(to be assigned)
515	Pair production, electron field

MT	Description
516	Pair production, nuclear and electron field (i.e., pair plus triplet production)
517	Pair production, nuclear field
518	Photofission (γ,f)
519-531	(to be assigned)
532	Photoneutron (γ,n)
533	Total photonuclear
534-601	(to be assigned)
602	Photoelectric
603-699	(to be assigned)
700	(n,p_0) cross section (cross section for leaving the residual nucleus in the ground state).
701	(n,p_1) cross section for first excited state
702	(n,p_2) cross section for second excited state
703	(n,p_3) cross section for third excited state
704	(n,p_4) cross section for fourth excited state
.	
.	
.	
718	(n,p_c) cross section for continuum excited state
719	(n,p_c') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing proton).
720	(n,d_0) cross section for ground state
721	(n,d_1) cross section for first excited state
722	(n,d_2) cross section for second excited state
.	
.	
.	
738	(n,d_c) cross section for continuum excited state
739	(n,d_c') cross section for continuum specifically not included in σ total (redundant, used for describing outgoing deuteron).
740	(n,t_0) cross section for ground state

MT	Description
741	(n,t_1) cross section for first excited state
742	(n,t_2) cross section for second excited state
•	
•	
•	
750	(n,t_c) cross section for continuum excited state
759	(n,t_c') cross secton for continuum specifically not included in σ total (redundant, used for describing outgoing triton).
760	$(n,^3He_0)$ cross section for ground state
761	$(n,^3He_1)$ cross section for first excited state
•	
•	
•	
778	$(n,^3He_c)$ cross section for continuum
779	$(n,^3He_c')$ cross section for continuum specifically not included in σ total (redundant, used for describing outgoing ^3He)
780	(n,α_0) cross section for ground state
781	(n,α_1) cross section for first excited state
•	
•	
•	
798	(n,α_c) cross secton for continuum
799	(n,α_c') cross section for continuum specifically not included in σ_T (redundant, used to describe outgoing α)
800-999	(to be assigned)

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