MACK

M.A. Abdou, C.W. Maynard, and R.Q. Wright

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M.A. Abdou, C.W. Maynard, and R.Q. Wright

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

http://fti.neep.wisc.edu

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MACK: A PROGRAM TO CALCULATE NEUTRON ENERGY RELEASE PARAMETERS (FLUENCE-TO-KERMA FACTORS) AND MULTIGROUP NEUTRON REACTION CROSS SECTIONS FROM NUCLEAR DATA IN ENDF FORMAT

M. A. Abdou
C. W. Maynard
R. Q. Wright

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TABLE OF CONTENTS

ABSTRACT

A model for calculating neutron energy release parameters (fluence-to-kerma factors) is discussed. The computer program MACK designed to calculate pointwise neutron fluence-to-kerma factros from nuclear data in ENDF format is described.

MACK calculates the following: (1) pointwise cross sections at an arbitrary energy mesh, (2) cross sections from resonance parameters in the resolved and unresolved resonance region, (3) energy group cross sections by reaction, (4) pointwise kerma factors, and (5) multigroup kerma factors. The energy point mesh and group structure can be arbitrarily set by the user. Kerma factors and cross sections can be averaged over an arbitrary input weighting function or any of several built-in functions.

The kerma factors and cross sections by reaction are of prime importance in calculating heating rates, dose and reaction rates of interest in any nuclear system.

COMPUTER CODE ABSTRACT

1. Name: MACK[1]

2. Computer: MACK is designed to operate on the UNIVAC-1108 and the IBM-360 series.

3. Problems Solved: The principal purpose of the program is in calculating pointwise neutron energy release parameters (fluence-to-kerma factors) at an arbitrary energy mesh from nuclear data in ENDF/B format[2]. The kerma factors are of prime importance for calculating heating rates and dose in any nuclear system. The program processes all reactions significant to energy deposition. In addition, the program calculates energy group kerma factors and group cross sections by reactions (group constants not transfer matrices) averaged over an arbitrary input weighting function or any of the "built-in" functions. When resonance data is available, the code calculates the contribution from the resolved and unresolved resonance parameters. The pointwise cross sections, pointwise kerma factors, energy group cross sections and energy group kerma factors can be printed, punched, and/or saved on tape for all reactions and the sum as selected by input. The pointwise kerma factors can be saved for later use[3] to generate group kerma factors for a different energy group structure and for inclusion in the ENDF/B evaluation for the nuclide with the appropriate MT numbers in the 300's series[2].

4. Method of Solution: The expressions for the energy release

per reaction are obtained from a solution of the kinematics of nuclear reactions. The anisotropy of elastic and inelastic scattering is included. The contribution to energy deposition from radioactive decay of the residual nucleus can be added by reaction and is calculated using Fermi theory in the case of β-decay. In the resolved resonance region, MACK accepts either single or multi-level Breit-Wigner parameters. Doppler broadening is performed at an arbitrary input temperature. The unresolved resonance treatment includes some shielding effects through a $1/\sigma_t$ weighting. The energy group kerma factors and cross sections are calculated by averaging the pointwise data over either a user supplied input specturm or "built-in" weighting functions. The program calculates the contribution to the energy release from all reactions and the accuracy of the kerma factors calculation is set only by the availability of the required nuclear data.

5. Restrictions on the Complexity of the Problem: Because of the variable dimensioning technique used in the program, the principal restriction on the size of the problem is the availability of sufficient core storage. Problems with up to about 1500 energy points can be run in less than 65 K words of core storage. Core storage requirements are not affected by the number of reactions processed for the nuclides nor the number of nuclides in a run. The code recognizes almost all of the multiplicity of data formats allowed by ENDF/B.

6. Typical Machine Time: Running time depends on a) number of resonances, b) Doppler broadening, c) size of the energy mesh selected for calculating the pointwise kerma factors, d) number of groups, and e) number of reactions processed. For nuclides with no resonance data, the typical running time is approximately 2 to 3 minutes on the UNIVAC-1108 for 1000 energy points and 100 groups. The running time for nuclides with resonance data depends strongly on the number of resonances and Doppler broadening and varies from 3 to 15 minutes on the UNIVAC-1108. Running times quoted are lower by approximately a factor of 4 for the IBM 360/91.

7. Unusual Features of the Program: MACK is the first code to calculate neutron fluence-to-kerma factors from nuclear data in ENDF format.

8. Related and Auxiliary Programs: Since the code has a "built-in" resonance treatment and recognizes all of the multiplicity of ENDF/B data formats, it does not depend on any other code. Only a nuclear data library in ENDF/B format is required.

9. Status: MACK is in production use on the UNIVAC-1108 at the University of Wisconsin and on the IBM 360/75/91 by individuals at ORNL.

10. References:

1. M. A. Abdou, C. W. Maynard, and R. Q. Wright, "MACK: A Computer Program to Calculate Neutron Energy Release Parameters (Fluence-to-Kerma Factors) and multigroup Neutron Reaction Cross Sections from Nuclear Data in ENDF Format" ORNL-TM-3994 (this report).

2. M. K. Drake, Editor, "Data Formats and Procedure for the ENDF Neutron Cross Section Library," BNL-50279 (October 1970).

3. M. A. Abdou and R. W. Roussin, "MACKLIB: Neutron Fluence-to-Kerma Factor Library Generated with MACK from Nuclear Data in ENDF Format," ORNL-TM-3995.

11. Machine Requirements: Approximately 65 K words of core storage. One scratch tape or disk is always needed in addition to the standard I/ϕ devices. One or two additional tapes may be needed depending on the characteristics of the problem[1].

12. Programming Language Used: MACK is programmed in standard FORTRAN-IV.

13. Operating System: UNIVAC-1108, EXEC-8 and IBM OS 360 with FORTRAN H Compiler.

14. Programming Information: The program presently consists of about 5700 FORTRAN statements in 69 subroutines. A 4-segment overlay structure is presently used.

15. User Information: The code and report can be obtained through the Radiation Shielding Information Center (RSIC) at ORNL.

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I. INTRODUCTION

Calculation of the heat-generation rate and dose due to interaction of nuclear radiation with matter is of prime importance in practically any nuclear system.

For the purposes of calculation, the heating rate due to neutron reactions with nuclei of the target material is divided into two types of contribution; the first type is heat generated by neutron reactions, and the second is heat generated by secondary gamma-radiation produced by these neutron reactions. As an example, consider the (n,p) reaction. The energy deposited of the first type is the kinetic energy of the recoil nucleas, the proton emitted and of any charged particle (e.g. β^-) which may be emitted from the activated residual nucleas. The energy deposition by the gamma-photons emitted is treated separately.

Heating by neutrons at any spatial point can be expressed as

$$H(r) = \int \phi(\vec{r},E) \sum_j \sum_i N_j(\vec{r}) \sigma_{ij}(E) E_{ij}(E) dE \ (eV/cm^3 sec). \quad (1.1)$$

where

$\phi(r,E)$ = neutron flux at spatial point r and energy E,

$N_j(\vec{r})$ = number density of element j at point r, $(atoms/cm^3)$

$\sigma_{ij}(E)$ = microscopic cross section of element j for reaction i at neutron energy E $(cm^2/atom)$

$E_{ij}(E)$ = energy deposited per reaction i in element j (eV).

The units have been chosen as those normally employed in nuclear calculations.

The terms k_{ij} and Kj defined as

$$k_{ij}(E) = \sigma_{ij}(E) E_{ij}(E) \quad (1.2)$$

$$k_j(E) = \sum_i k_{ij}(E) \quad (1.3)$$

are flux and density independent. Hence, the heating rates can be calculated from particle transport results for any system if the factors k_j are predetermined for all materials in the system.

k_{ij} is called the microscopic kerma factor for reaction i in element j. The term "kerma" is an acronym standing for the Kinetic Energy Released in Materials. The phrase "fluence-to kerma factors" was introduced by the International Commission on Radiological Units and Measurements [1]. The term "kerma" will be used throughout this report as defined by equations 1.2 and 1.3 on the previous page, with E_{ij} as defined next.

$E_{ij}(E)$ is the energy released in element j per reaction i induced by a neutron of energy E. The energy release considered here is the energy which can be assumed to be deposited locally, i.e., within a negligible distance from the site of the reaction. This implies that E_{ij} is the sum of the kinetic energies of the recoil nuclei, charged particles emitted, and charged particles produced by radioactive decay of the residual nucleas and such other processes as internal conversion. The addition of the contribution from radioactive decay to energy deposition depends on the type of calculation performed, time dependent or steady state. This comment will be elaborated on later.

The gamma-ray kerma factors are defined in a similar manner and can be determined from

$$k_\gamma^j = \sigma_{pe}^j E + \sigma_{pp}^j (E-1.02) + \sigma_{ca}^j E \qquad (1.4)$$

where

$k_\gamma^j(E)$ = gamma kerma factor for element j (MEV.cm^2/atom)

E = photon energy (MeV)

σ_{pe}^i = photoelectric microscopic cross section for element j (cm^2/atom)

σ_{ca}^{j} = Compton microscopic absorption cross section for element j (cm^2/atom)

σ_{pp}^{j} = pair production microscopic cross section for element j (cm^2/atom)

In pair production, 1.02 MeV (two electron masses) of the photon energy is not available for local heat disposition. The two .51 MeV photons produced by the pair are accounted for in the transfer cross sections of gamma energy multi-group cross section sets, hence the energy balance is maintained. Implicit in the use of Eq. (1.4) is the assumption that photoelectric, pair production, and Compton scattering are the only processes that contribute to energy desposition, thus all other possible processes are assumed negligible.

The evaluation of gamma kerma factors (Eq. (1.4)) is straightforward and is usually performed by the codes which generate multigroup photon cross sections such as MUG[8] and GAMMA[9]. Therefore, gamma kerma factor calculations present no problem at present.

Calculation of neutron kerma factors, on the other hand, is complicated by the variety of reactions which a neutron can undergo, and the emission of more than one particle in many of these reactions. However, the kinematics and theory are still simple and the limitation on the accuracy of a neutron kerma calculation is set by the availability and accuracy of the nuclear data.

Prior to the work reported here there were several efforts at calculating kerma factors. Some of these are reported in references [2-7]. However, these efforts were directed mostly toward calculating kerma for elements which are major constitutents in the human body. Furthermore, they involved several simplifying assumptions such as neglecting inelastic scattering entirely, anisotropy of elastic scattering,

and several others. The work of Ritts et. al [6] included a larger number of reactions and was certainly an improvement over all preceeding work. They calculated kerma factors for 11 elemental constitutents of the human body. This work was extended [7] to calculate kerma for seven elements of interest in fusion reactor blankets. However, Ritts et. al. in their work did not have a general format or algorithm for calculating kerma and the same effort had to be duplicated for each material or for a new evaluation of the basic data for the same material. In addition, it involved some approximations in calculation of the secondary neutron energy distribution and the excitation of residual nuclei in non-elastic reactions.

The Evaluated Nuclear Data File(ENDF)[10] provides a unified format that is used to store and retrieve evaluated sets of neutron and photon cross sections. The ENDF formats are versatile and flexible enough that almost any type of neutron interaction mechanism can be accurately described. Further, the nuclear data in the ENDF/B library is continously revised, re-evaluated, and updated. Thus, it provides the most suitable up-to-date nuclear data library.

The computer program MACK was developed for calculating neutron-induced kerma factors from nuclear data in ENDF/B format. The generality of the ENDF/B format requires a greater generality on the part of any processing code which utilizes this data. In addition, it is expected that modifications and improvements in the data representation in ENDF/B will frequently be made. The MACK program accomodates the ENDF/B format generality and the programming is transparent enough that any necessary changes can easily be made.

The basic purpose of the MACK program is to calculate neutron-induced kerma factors as a function of neutron energy. The calculation is carried out for a discrete energy mesh flexibly specified by input options for any desired energy range. In addition, several calculational routines were included in the program to generate energy group kerma factors and energy group cross sections (group constants, not transfer matrices) for any reaction type desired. These options provide a rapid and economical way of obtaining cross sections in multigroup form for calculation of reaction rates of interest; e.g., helium, hydrogen and tritium production. The MACK code also has a built-in resonance treatment and the resonance cross sections can be computed, Doppler-broadened at an arbitrary temperature, from resonance parameters (ENDF/B file 2). This provides the code with independence from other programs in processing ENDF/B data for resonance nuclides.

The remainder of this report is divided into four sections. The theory for neutron-induced kerma factor calculation is briefly discussed in Section II. In Section III, the models for processing nuclear data in ENDF/B format are discussed. MACK input and output are explained in Section IV. Section V is a collection of useful user-information.

II. THEORY FOR KERMA FACTOR CALCULATIONS

The macroscopic kerma factor for an element j was defined in the introduction to be

$$k_j = \sum_i k_{ij} \qquad (2.1)$$

$$k_{ij}(E) = \sigma_{ij}(E)\, E_{ij}(E) \qquad (2.2)$$

where

E = incident neutron energy (eV)

$\sigma_{ij}(E)$ = microscopic cross section of element j for reaction i at incident neutron energy E (cm^2/atom)

$E_{ij}(E)$ = energy released per reaction i in element j (eV)

From the above equations, it is clear that the basic quantity to be calculated for generating kerma factors is the energy released by each type of reaction, E_{ij}, and this is the subject of this section.

Since we need to consider only kerma for an element, the subscript j will be dropped from here on. Furthermore, since one reaction will be considered at a time in the following discussion, the subscript i will also be dropped unless a distinction is needed. Throughout this section, several quantities will be used as defined below (for each reaction)

E_r = kinetic energy of the recoil nucleas

E_R = sum of kinetic energies of recoil nucleas and charged particles emitted.

E_H = total energy release from the reaction considered ($E_H = E_{ij}$)

A = AWR = ratio of the nuclear mass of the element to that of the neutron.

Reaction Types

For kerma calculation, the nuclear reactions are conveniently classified

into the seven types given in Table 1. In Table 1, MT is the ENDF/B reaction number and LR is a flag used in ENDF/B3 to allow inclusion of information about the (n,n') part of a combined inelastic reaction (other than γ-ray emission) by presenting these reactions with MT = 50-91 (inelastic scattering to levels and continuum) and using the appropriate MT number in the LR flag field.

The methods used to calculate the energy released by each type of reaction are summarized below. The kinematics are derived from energy and momentum conservations; however, the details are not given here.

Since ENDF data generally extends only to 15 MeV at present, which is the energy range required for most applications, contributions to the kerma factors from (n,3n) reactions and from secondary nuclear reactions caused by charged particle products of the primary reaction are neglected.

Elastic Scattering

The only contribution to kerma elastic scattering is the deposition of the kinetic energy of the recoil nucleas, E_r; i.e.

$$E_H = \bar{E}_r \qquad (2.3)$$

E_r is a function of the scattering angle of the neutron. The average recoil energy is obtained by weighting $E_r(\theta)$ by the differential scattering cross section.

$$\bar{E}_r = \frac{2AE}{(A+1)^2} \quad (1 - \overline{\cos \theta_{cm}}) \qquad (2.4)$$

Table 1

REACTION TYPES

For the Purpose of Kerma Calculation, The Nuclear Reactions are Classified Into the Following Types

	REACTION TYPE	MT
1- (n,n)	Elastic	2
2- (n,n')γ	Inelastic Level	51-90
3- (n,n')γ	Inelastic Continuum	91
4- (n,mn')a_{c_1},a_{c_2} ...	(n,mn') Charged Particles	22,23,24,28 and
	m = 1 or 2	51-91 with Flag LR
5- (n,a_{c_1} ,a_{c_2} ,a_{c_3} ...)	(n, Charged Particles)	103-109 700-799
6- (n,γ)	Radiative Capture	102
7- (n,2n)		16

where

$\overline{\cos(\theta_{cm})}$ = average of the cosine of the center-of-mass scattering angle.

$$\cos(\theta) = \frac{\int_{-1}^{+1} \mu\sigma(\mu,E)d\mu}{\int_{-1}^{+1} \sigma(\mu,E)d\mu} = F_1 \qquad (2.5)$$

where

$\mu = \cos\theta$

F_1 = first coefficient of the Legendre polynomial expansion of the differential scattering cross section.

Inelastic Level Scattering

The average energy of the recoil nucleas is given by

$$\bar{E}_r = E - \bar{E}_{n',1} - E_\lambda \qquad (2.6)$$

where

E = incident neutron energy

E_λ = energy of the excited level

$\bar{E}_{n',1}$ = average kinetic energy in the laboratory system of the emitted neutron

$\bar{E}_{n',1}$ is given by

$$\bar{E}_{n',1} = \frac{2AE}{(A+1)2}\left[\frac{A^2+1}{2A} - \frac{(A+1)E_\lambda}{2E} + \sqrt{1 - \frac{A+1}{A}\frac{E_\lambda}{E}}\,\overline{\cos\,\theta}_{cm}\right] \qquad (2.7)$$

where

$\overline{\cos\ \theta}$ = average of the cosine of the scattering angle in the center-of-mass,

A = atomic weight of the particular isotope (if the material considered is a mixture of isotopes) in which the level considered is excited.

The energy deposition per inelastic level reaction can be written as:

$$E_H = \bar{E}_r + f_c E_\lambda \qquad (2.8)$$

f_c is the fraction of E_λ converted to heat. For example, if internal conversion competes with γ-emission, then f_c is biven by

$$f_c = C_F/(1+C_F) \qquad (2.9)$$

where

C_F = internal conversion factor

(n,n')γ to the continuum

Here the average recoil energy is given by

$$\bar{E}_r = E - \bar{E}_{n',1} - \bar{\varepsilon} \qquad (2.10)$$

where

$\bar{\varepsilon}$ = average excitation of the residual nucleas

$$\bar{\varepsilon} = \frac{A^2+1}{A(A+1)} E - \frac{A+1}{A} \bar{E}_{n',1} \qquad (2.11)$$

and $\bar{E}_{n',1}$ = average kinetic energy of the secondary neutron emitted in the laboratory system.

The energy distribution of the secondary neutron, $P(E\to E')$, can be broken down into partial energy distribution $f_k(E\to E')$, where each of the partial distributions can be described by different analytic representations

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

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 $\bar{E}_{n',1}$ is evaluated as follows

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

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

$$= \sum_{k=1}^{NK} P_k(E) \, \bar{E}_{n',l,k} \qquad (2.12)$$

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

For the evaporation spectrum,

$$f(E\to E') = \frac{E'e^{-E'/\theta(E)}}{I}$$

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

$$\bar{E}_{n',l,k} = \theta \frac{2e^{x_1} - \{1+(1+x_1)^2\}}{e^{x_1} - (1+x_1)} \qquad (2.13)$$

where

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

For a simple fission spectrum (Maxwellian)

$$f(E\to E') = \frac{\sqrt{E'}}{I} e^{-E'/\theta(E)} \qquad (2.14)$$

and invoking the assumption that $E'_{min} = 0$, there results

$$\bar{E}_{n',l,k} = \theta \left[\frac{3}{2} - \frac{x_1^{3/2}}{\{\frac{\sqrt{\pi}}{2} e^{x_1} \operatorname{erf}(\sqrt{x_1}) - \sqrt{x_1}\}} \right] \qquad (2.15)$$

The other allowable representations for $f_k(E \rightarrow E')$ in ENDFB are discussed in a later section.

(n,n') Charged Particles

In this type of reaction, in addition to the secondary neutrons, the emission of one or two charged particles occurs. The reaction is generally of the form

$$Z_1X^{A_1}(n,n')a_{c_1}, a_{c_2}, \ldots\ldots a_{c_n}, Z_2Y^{A_2}$$

Define

$$E_R = E_r + E_{a_{1_c}} + E_{a_{2_c}} + \ldots + E_{a_{n_c}} \qquad (2.16)$$

where

E_r = kinetic energy of recoil nucleas Y

$E_{a_{i_c}}$ = kinetic energy of the i^{th} charged particle

In kerma calculation, we are not concerned with the partition of energy between charged particles and the recoil nucleas since all charged particles (and the "recoil nucleas") will deposit their kinetic energy at or near the site of collision. This allows the evaluation of E_R applying only the energy conservation principle

$$\bar{E}_R = E - \bar{E}_{n',1} - |Q_o| - \varepsilon_Y \qquad (2.17)$$

where

$\bar{E}_{n',1}$ = average energy of the neutron emitted in the laboratory system

Q_o = Q-value for the combined reaction when the residual nucleas is left in the ground state,

ε_Y = average excitation of the residual nucleas

Assuming that in an $(n,n')a_{c_k},a_{c_2}\ldots a_{c_n}$ type reaction the neutron is emitted first, $\bar{E}_{n',1}$ can be evaluated as discussed before for inelastic to discrete or continuum level scattering depending on the state of the intermediate nucleas left after the emission of the neutron.

If the residual nucleas, after emitting the neutron and charged particles, is left in the isolated level region, E_R and the corresponding kerma factor must be evaluated for each possible level. If the residual nucleas is left in the continuum range (infrequent for reactions induced by neutrons of energy less than 14 MeV), the evaluation of the average energy of the residual nucleas requires information about the energy spectra of the charged particles emitted. Currently, ENDFB does not provide such information.

In reactions of the type $(n,2n)a_{c_1},a_{c_2}\ldots a_{c_n}$; E_R can be evaluated from the last equation with $\bar{E}_{n',1}$ as the sum of the average energies of the two neutrons.

The total energy release per reaction, E_H, is the sum of E_R and E_{decay} where E_{decay} is the contribution to heat deposition by particle emission (usually β^- or β^+) from the decay of the activated residual nucleas. Methods for calculating E_{decay} will be given after discussing the kinematics of the other types of reactions.

Charged Particle Reactions

The reaction discussed here is of the type

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

where a_{c_1},a_{c_2} ... are charged particles; e.g. (n,α), (n,p), $(n,\alpha T)$. The partition of the kinetic energy of the emitted charged particles and the residual nucleas is not needed.

$$E_H = E_R + E_{decay}$$

where

$$E_R = E_{a_{c_1}} + E_{a_{c_2}} + E_{a_{c_n}} + E_r$$

The residual nucleas is frequently left in one of the excited states and the kerma factor for this type of reaction is the sum of the kerma factors to each level, i.e.

$$k = k_0 + k_1 + k_2 + ... + k_N + k_{con} \qquad (2.18)$$

where N is the number of levels and the subscript con denotes continuum.

Denoting E_R, and E_H for the i^{th} level by E_{Ri} and E_{Hi} respectively, we can write

$$E_{Ri} = E + Q_o - \varepsilon_{Yi} \qquad (2.19)$$

where

Q_o = reaction mass Q-value (Q-value to the ground state)

ε_i = energy of level i excited in the residual nucleas.

The quantities E_{Hi} and k_i are

$$E_{Hi} = E_{Ri} + E_{di} \qquad (2.20)$$

and

$$k_i = \sigma_i E_{Hi} \qquad (2.21)$$

where σ_i = reaction cross section for the i^{th} excited state,

and E_{d_i} = contribution to energy deposition by radioactive decay of the i^{th} level (except γ emission)

The expression for k can be easily expressed as

$$k = \sigma[(E + Q_o) - E_\gamma + E_{decay}] \qquad (2.22)$$

where

$$E_\gamma = P_1\varepsilon_1 + P_2 \varepsilon_2 + ... + P_N\varepsilon_N \qquad (2.23)$$

$$E_{decay} = P_0 E_{d0} + P_1 E_{d1} + \ldots + P_N E_{dN} \qquad (2.24)$$

and

ε_i = energy of the i^{th} level

P_i = probability that the i^{th} level will be excited given that a reaction has occurred.

If other processes compete with γ emission, the ε_i's in the above expression should be adjusted. For example, if internal conversion competes with γ emission from the i^{th} level, then ε_i should be adjusted to

$$\varepsilon_{im} = \varepsilon_i (1-f_c) \qquad (2.25)$$

with

$$f_c = C_F/(1+C_F) \qquad (2.26)$$

where C_F = internal conversion factor.

Radiative Capture

The kinetic energy of the recoil nucleas in an (n,γ) reaction is obtained by momentum and energy balance which yield

$$E_r = E + Q + M_r c^2 - M_r c^2 \sqrt{1 + \frac{2(Q+\frac{AE}{A+1})}{M_r c^2}} \qquad (2.27)$$

where

Q = the reaction Q-value

A = ratio of the nuclear mass of the target nucleas to that of the neutron

$M_r c^2$ = mass of the residual nucleas in energy units
$= (A+1)m_n c^2 - Q$

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

If radioactive decay occurs after an (n,γ) reaction E_H is the sum of E_r and E_{decay}.

(n,2n) Reaction

(n,2n) reactions followed by charged particle emission were treated previously. We are concerned here with (n,2n) reactions followed by γ emission (or internal conversion). The recoil energy of the nucleas is given by

$$\bar{E}_r = E - (\bar{E}_{n_1,1} + \bar{E}_{n_2,1}) - B - \bar{\varepsilon}_{A-1} \qquad (2.28)$$

where

$\bar{E}_{n_1,1}$ = average kinetic energy of first neutron emitted in the laboratory system

$\bar{E}_{n_2,1}$ = average kinetic energy of second neutron emitted in the laboratory system

B = binding energy of the last neutron in the target nucleas

$\bar{\varepsilon}_{A-1}$ = average excitation of the residual nucleas

Assuming that the (n,2n) reaction is a two-step process, i.e. one neutron followed by another, $\bar{\varepsilon}_{A-1}$ can be shown to be

$$\bar{\varepsilon}_{A-1} = \frac{A^2+2}{A(A+1)} \; E - B - \frac{1}{A-1} \left[\frac{A^2-2}{A} \bar{E}_{n_1,1} + A \bar{E}_{n_2,1} \right] \qquad (2.29)$$

The average energy of each neutron can be calculated from the energy distribution of that neutron as was done previously. Evaluation of $\bar{\varepsilon}_{A-1}$ requires knowledge of the energy distribution for each of the two neutrons. If only the combined energy spectrum of the two neutrons is known, the calculation of $\bar{E}_r$ without approximation is possible only when the residual nucleas is left in the ground state.

The contribution to the energy deposition from internal conversion and radioactive decay - if any - should be added to $\bar{E}_r$ to get E_H.

Kerma Factors for a Mixture of Isotopes

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

$$K_m = \sum_j K_j \qquad (2.30)$$

and

$$K_j = N_j k_j \qquad (2.31)$$

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. Mo, Fe, etc.) which consist of several isotopes to directly evaluate the kerma factors for the element without calculation of 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 equation 2.30. 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, then by definition

$$\text{Q-value for the } j_{th} \text{ isotope} = Q_j = E_{R_j} - E \qquad (2.32)$$

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

$$N_m \sigma_m E_{R_m} = \sum_j N_j \sigma_j E_{R_j} \qquad (2.33)$$

where E_{R_m} is the kinetic energy of the produce 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 rewrite Eq. 2.33 as

$$E_{R_m} - E = \sum_j Q_j \frac{\sigma_j N_j}{\sigma_m N_m} \qquad (2.34)$$

Since the left hand side of equation 2.34 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.,

$$Q_m = \sum_j Q_j \frac{\sigma_j N_j}{\sigma_m N_m} \qquad (2.35)$$

Since definition (2.35) is derived by using only a conservation principle Eq. (2.33) 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

$$\bar{E}_{n',l,m} = \sum_j \frac{N_j \sigma_j}{N_m \sigma_m} \bar{E}_{n',l,j} \qquad (2.36)$$

and

$$E_{decay,m} = \sum_j \frac{N_j \sigma_j}{N_m \sigma_m} E_{decay,j} \qquad (2.37)$$

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 Equation 2.30. This is no surprise since kerma itself is a physical quantity and Equation 2.30 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. 2.30.

A special case implicitly included in Eq. 2.35-2.37 is a reaction which occurs only in one isotope. In this case, Eq. 2.36 reduces to

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

where J is the isotope in which this reaction occurs. An example is inelastic level scattering where each level belongs to a particular isotope. Therefore, in applying Eq. (2.7) 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-value, 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 in and the abundance of the constituent isotopes.

Energy Deposition Due to Radioactive Decay

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-life time for decay decreases rapidly as the disintegration energy increases. The contribution from activated residual nuclei with a mean life time greater than a few days is usually neglibly small. Thus, kerma factors in which radioactive decay is considered only for half-lives less than an arbitrary cut-off (e.g. 10 days) is suitable for steady state heating rate calculations. If the heating rate is to be calculated for a short period of operation of the nuclear system (e.g. start-up), 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 β particles. β^+ decay may occur after (n,2n) reactions and β^- after (n,γ) and (n, charged particles) reactions. Since β particles are emitted with an energy spectrum, the average kinetic energy of β particles, $\bar{E}_\beta$ must be calculated. Previous works[6,7] assumed the average kinetic energy of a β particle to be 30% of the end-point for all

isotopes and end-point energies. This assumption severely underestimates $\bar{E}_\beta$.

The basic problem in calculating $\bar{E}_\beta$ is the calculation of the energy distribution of the β-particles. Fermi's theory [12,13] of β decay predicts the probability of emitting a β-particle with kinetic energy E for endpoint energy E_0 to be

$$P(W) = GF(Z,W)(W^2-1)^{1/2}(W_0-W)^2W \qquad (2.38)$$

where,

$$W = \frac{E(MeV)}{0.51} + 1, \qquad (2.39)$$

$$W_0 = \frac{E_0(MeV)}{0.51} + 1$$

Z is the atomic number, and G is a quantity independent of W and its actual magnitude is not important in the following discussion. F(Z,W) is a complicated function which accounts for the effect of the nuclear coulomb potential on the emitted β-particle. The form of the F factor is discussed in Reference 12 and 13 and more detailed references are listed there. A relativistic expression for F is given as

$$F(Z,W) = \left\{\frac{4(1+s/2)}{[\Gamma(3+2s)]^2}\left(\frac{2r}{\hbar/m_oc}\right)^{2s}\right\}\left\{(W^2-1)^s e^{\pi y}\ |\Gamma(1+s+iy)|^2\right\} \qquad (2.40)$$

where

$$S = \left[1-\left\{\frac{Z}{137}\right\}^2\right]^{1/2} - 1 \qquad (2.41)$$

r = nuclear radius

$\hbar/m_oc = 3.86 \times 10^{-11}$ cm

Γ = complex gamma function

$$y = \frac{aZW}{137\sqrt{W^2-1}} \qquad \begin{cases} a = +1 \text{ for } \beta^- \text{ decay} \\ a = -1 \text{ for } \beta^+ \text{ decay} \end{cases} \qquad (2.42)$$

For $|s|<<1$, $F(Z,W)$, to a good approximation, is given by

$$F(Z,W) \simeq \frac{2\pi y}{1-e^{-2\pi y}} \qquad (2.43)$$

with y as given in Eq. (2.42)

The average energy of a β particle, $\bar{E}_\beta$, can be written as

$$\bar{E}_\beta(\text{MeV}) = 0.51 \frac{\int_1^{Wo} (W-1)P(W)dW}{\int_1^{Wo} P(W)dW} \qquad (2.44)$$

with P(W) given by Eq. (2.38) and F(Z,W) by Eq. (2.40). The nonrelativistic appriximation, Eq. 2.43, has less than 2 per cent error in evaluating $\bar{E}_\beta$ for Z<40. For Z = 0, F(Z,W) is unity.

Eq. (2.44) was evaluated numerically using Eq. (2.43) for F(Z,W) and the results are tabulated in Appendix C for a wide range of Z and E_0 for both β^- and β^+. The ratio, R, of $\bar{E}_\beta$ to the endpoint energy is also tabulated. Several conclusions can be drawn from investigation R.

The results show that R is generally an increasing function of E_0 and is always greater than 30% for E_0 greater than about 0.5 MeV. It increases rapidly with E_0 and Z up to an E_0 of about 3 MeV after which it varies more slowly. In Figure 1, R is plotted as a function of E_0 for Z = 30 for β^- and β^+ compared with R for Z = 0 for which the coulomb correction is not included. Figure 1 and the tabulated results in Appendix C show that for each endpoint energy R decreases for β^- and increases for β^+ when the nuclear coulomb effect is taken into consideration. The change in R for both β^- and

β^+ is more pronounced at smaller E_0. These observations can be explained as follows. The nuclear coulomb potential represents a potential well for the electrons and a barrier for the positrons. Therefore, in β^- decay a surplus of low-energy electrons is produced resulting in a lower R. For β^+ decay, F(Z,W) of Eq. 2.43 is $\simeq 2\pi|y|e^{-2\pi|y|}$ for low-energy positrons. This is a typical barrier transmission factor. Since $|y|$ increases as Z increases and E decreases (Eq. 2.42) the nuclear coulomb effect is most noticable at high Z and low E. The barrier transmission factor nearly eliminates the emission of low-energy positrons resulting in a higher R. At very low E_0 the β^+ spectrum is almost non-zero only in the neighborhood of E_0 and therefore, R approaches unity as E_0 tends to zero.

$\bar{E}_\beta$ for a given E_0 and Z can be obtained by linear interpolation of R in tables of Appendix C. For isotopes with two or more β spectra with different endpoint energies, $\bar{E}_\beta$ must be calculated separately for each spectrum and summed weighted by the intensities.

As an example of calculating the contribution to the kerma factor from radioactive decay consider radiative capture in Li^7.

$$Li^7(n,\gamma)Li^8 \xrightarrow[T_{1/2} = .84\,S]{\beta^-} Be^8 \Longrightarrow 2\alpha$$

Li^8 decays by a 100% intensity β spectrum to the 2.90 MeV level of βe^8 which disintegrate immediately to two α particles. Q_{β^-} and Q_α are calculated as 16.002 and 0.095 MeV respectively. Hence, the endpoint β kinetic energy is 13.102 and each α particle has kinetic energy equal to 1.497 MeV. From results in Appendix C for Z = 3, we get $\bar{E}_\beta$ = 6.315 MeV. Hence, the contribution from radioactive decay per (n,γ) reaction in Li^7 is 9.31 MeV. Incidentally, the Q-value for the (n,γ) reaction in Li^7 is 2.032 MeV, and thus

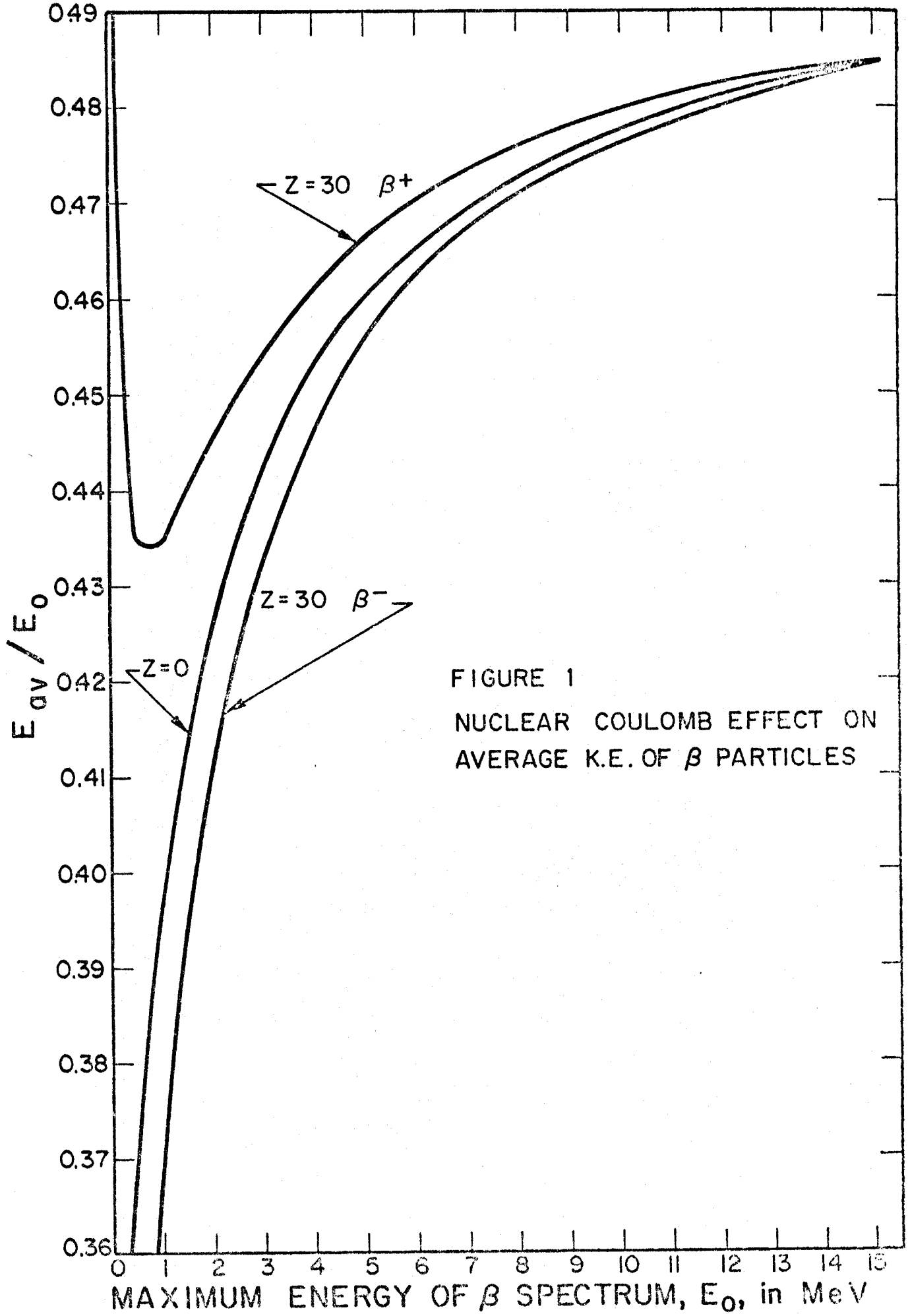


FIGURE 1

NUCLEAR COULOMB EFFECT ON AVERAGE K.E. OF β PARTICLES

the kerma factor for that reaction is dominated by the contribution from the decay of the activated residual nucleas.

The average energy of β decay is not usually given in the table of isotopes [14] nor in other compilations of radioisotopes. The β endpoint energy, relative intensities, fraction of electron capture, α-particle energies, half-lives and other required information are usually given in such compilations. This suggests generating a library for the average energy release from radioactive decay for all reactions and isotopes of importance. Such a library will not be only useful for adding the contribution of radioactive decay to kerma factors but also will provide necessary information for calculation of decay heat in nuclear devices. It is also suggested that the average energy release fron radioactive decay following a nuclear reaction be specified in ENDF/B file 1 section 453.

The MACK code provides several options for adding the energy release contribution of radioactive decay that follows a nuclear reaction to the energy release calculated from recoil of charged particles. These options are fully described in the input description section given later.

A final point worth mentioning is about the contribution to energy release by gamma emission from radioactive decay. Since the gammas are frequently of high energy, they are transported through the medium away from the site of the neutron reaction and they do not contribute to the local energy deposition. The energy deposition by these gammas can be properly accounted for

by adding them to the secondary gamma production source. However, since this procedure would sometimes be troublesome, the MACK user has the option for adding the gamma decay contribution.

III. ENDF DATA PROCESSING

Nuclear data in ENDF/B format is processed by MACK according to the ENDF "file" order. MACK processes ENDF neutron interaction data files. These files are titled:

File 1 - General Information

File 2 - Resonance parameter data

File 3 - Neutron cross sections

File 4 - Angular distribution of secondary neutrons

File 5 - Energy distribution of secondary neutrons

File 6 - Energy-angular distributions of secondary neutrons

File 7 - Thermal neutron scattering law data

File 1 Data

The descriptive information (MT = 451) is read and printed as it provides a brief description and documentation of the evaluated data. AWR (atomic weight ratio) and LRP (a flag that indicates that resonance parameters are given in file 2) are read and stored.

File 2 Data

File 2 contains data for both resolved and unresolved resonance parameters. For materials that have resonance parameters in file 2, the cross sections calculated from the resolved and for unresolved resonance parameters must be added to the appropriate data in file 3 to get the correct cross sections for radiative capture, fission, elastic scattering and total.

Calculation of cross sections in the resonance region is generally an expensive process. An alternative, for codes such as

MACK that process ENDF data but whose basic purpose is not generating pointwise cross sections, is to read point cross sections for resonance nuclides from an input tape generated by codes such as SUPERTOG[16] of ETOX[17]. This procedure, however, has the obvious disadvantage of depending on another code of the same size or larger. Therefore, a resonance treatment was built into MACK. This resonance treatment was adapted from the well-developed techniques used in some ENDF processing codes (ref. 16-21). MACK also has an option that allows for by-passing the resonance calculations and reading point cross sections for the appropriate reactions in resonance nuclides from an input tape.

The calculation of pointwise cross sections in the resonance region in MACK is discussed in APPENDIX B. These calculations need to be carried out only if the resonance energy range is within the energy range (specified by input) for kerma and group cross section calculations.

The resolved resononance parameters given in single-level Breit-Wigner or multi-level Breit-Wigner representations are processed in MACK. An option is available to get Doppler broadened cross sections at an arbitrary input temperature. In the region of unresolved resonances, the program permits all the three formats of ENDF/B for specifying the average resonance parameters. The details of the resonance region treatment in MACK are given in APPENDIX B.

After all resonance cross sections are computed in both the resolved and the unresolved resonance region, point average cross

sections are calculated in subroutine RXSECT at the appropriate kerma energy mesh points and stored on a scratch device. These cross sections are read in and added to file 3 data later in subroutine SIGPR to obtain the final energy point cross sections.

File 3 Data

The smooth cross sections are read from file 3 and a new cross section set is formed at the energy mesh used for kerma calculation using ENDF/B interpolation schemes. For each reaction, the LR flag is read and stored together with the reaction MT number in order to properly identify the reaction type when the kerma calculation is performed. The reactions Q-values are also stored since they are of basic importance for kerma calculations.

The partial cross sections for charged particle reactions (700's series) are also processed and for each reaction (e.g. (n,p)) the following quantities are calculated

$$E_\gamma(E) = \frac{1}{\sigma} [\sigma_1 E_1 + \sigma_2 E_2 + \text{---} + \sigma_N E_N]$$

where σ_i = partial cross section for exciting i^{th} level

E_i = energy of the i^{th} level

σ = total reaction (e.g. (n,p)) cross section

An array of E_γ is calculated for each charged particle reaction ((n,p) , (n,d), etc.) since it is needed for kerma calculations for these reactions (see equation 2.22).

If energy group-averaged cross sections are desired by input option, they are calculated from file 3 data smooth cross sections and interpolation schemes using a straight forward average according to the prescription

$$\overline{\sigma}_{g,x} = \frac{\int_g W(E)\sigma_x(E)dE}{\int_g W(E)dE}$$

where x denotes the process; e.g., (n,γ), (n,α), etc.; g denotes the energy group, and W(E) is the weighting function.

The point cross sections are processed and generated in subroutine XSECN. The resonance contribution is added in subroutine SIGPR. Group cross sections are calculated in subroutine CROSG.

File 4 Data

File 4 contains representations of angular distributions of secondary neutrons, and in particular, the distributions for elastically scattered neutrons and for the neutrons resulting from discrete level excitation due to inelastic scattering. Angular distribution data is given in either:

1. Legendre coefficients in the CM (center of mass coordinate system),
2. Tabulated normalized probability distribution in the CM,
3. Legendre coefficients in the LAB (laboratory coordinate system),
4. Tabulated normalized probability distribution in the LAB system.

For elastic scattering, a transformation matrix may be given to be used to transform the data from one frame of reference to the other.

From the theoretical formulation given before, the average of the cosine of the scattering angle in the center-of-mass system for elastic and inelastic level scattering is needed in order to calculate the average kinetic energy of the recoil nucleas in each of these reactions. This is equal to the first coefficient of the Legendre polynomial expansion (in CM system) of the scattered neutrons. If data is given in the first form mentioned above, the

quantity needed is obtained directly by interpolation at the required energy points. For the second type of data, we use

$$\cos\ (\theta_{cm})_E = \int_{-1}^{+1} \mu P(\mu,E)d\mu$$

where $\mu = \cos(\theta_{cm})$

$P(\mu,E)$ = normalized probability distribution of the scattering direction cosine.

The third type is also processed. If the transformation matrix is given it is used, otherwise the code uses the approximation in the papers by Zweifel and Hurwitz[22] and Amster[23] to transform the data from LAB to CM system. The approximations work well only in the case

$$\gamma = \frac{1}{A}\sqrt{\frac{E}{E+Q(\frac{A+1}{A})}} < 1$$

For elastic scattering ($\gamma = \frac{1}{A}$) this condition is always met. However, for some cases of inelastic scattering (and usually for energies close to the threshold energy), this condition is not satisfied. The anistropy in nonelastic reactions is neglected at energies for which the condition is not met.

If data is given as tabulated probability distributions in LAB, Legendre coefficients in the LAB are generated and the treatment mentioned above is used to transform these coefficients into the CM system.

File 5 Data

File 5 contains data for energy distribution of secondary neutrons. The energy distributions are expressed as normalized probability distributions and can be broken down into partial energy distributions.

The partial energy distributions are represented by several forms, as designated by the "LF-number." The energy distribution laws currently allowed in ENDF/B are the following types:

A. LF = 1 Arbitrary tabulated function.

B. LF = 5 General evaporation spectrum.

C. LF = 7 Simple fission spectrum.

D. LF = 9 Evaporation spectrum.

E. LF = 10 Watt spectrum

MACK processes the average energy of the secondary nuetron for nonelastic reactions from file 5 as discussed below.

$$\overline{E}_{n',1}(E) = \frac{\int_{E'min}^{E'max} E'P(E\rightarrow E')\,dE'}{\int_{E'min}^{E'max} P(E\rightarrow E')dE'}$$

This can be written in the form

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

$$= \sum_{k=1}^{NK} P_k(E)\overline{E}_{n',1,k}$$

where NK is the number of partial energy distributions and

$$\overline{E}_{n',1,k}(E) = \int_{E'min}^{E'max} E'f_k(E\rightarrow E')dE'$$

The analytic formula for $\overline{E}_{n',1,k}$ depends on the analytic formulation (LF) number of $f_k(E\rightarrow E')$. Expressions for $\overline{E}_{n',1,k}$ for LF = 7 and LF = 9 were given earlier in Equations 2.13 and 2.15. $\overline{E}_{n',1,k}$ for LF = 1

is obtained by numerical integration of $E'f_k(E\rightarrow E')$. For partial distribution given as a general evaporation spectrum $f(E\rightarrow E')=g(E'/\theta(E))$, a new partial distribution $f(E\rightarrow E')=G(E\rightarrow E')$ is obtained and numerical integration is performed. The Watt spectrum (LF = 10) is not programmed into the code since its basic use is for fissionable materials and from a physics point of view it cannot be used in its present format to represent the energy distributions of secondary neutrons in nonelastic processes other than fission.

E'_{min} is specified by ENDF/B to be zero and for LF = 7 and LF = 9, E'_{max} = E-U where U is independent of energy. Those limits were used in the code. However, their usage results in an error in the calculation of the average energy of the secondary neutron and the average excitation of the residual nucleas. The laboratory energy of a secondary neutron can never be zero and the maximum is frequently not representable in the form E-U (with U independent of energy).

IV. INPUT AND OUTPUT DESCRIPTION

On the following pages, the input and output data for MACK are explained. The section is divided into three parts. Part A is a guide in preparing the input. Detailed data notes are given in Part B. Part C is a description of MACK output.

A. Input Description

This part is a brief description of the input data. Standard FORTRAN conventions used to describe the data formats and the program symbol name for each item are listed. The columns to be used for each data item are also designated.

Card No. 0 (2I6)

This card is always the first card in the input data. It is required only once in a single run and is not to be repeated for each material.

Item	Cols.	Name	Description
1	1-6	IDTAP	ENDF/B tape identification number.
2	7-12	MODE	Mode of ENDF/B data tape. 1 = binary tape 2 = BCD tape

The input data for each material is as follows.

Card No. 1 (18A4)

Title card.

Card No. 2 (I6,4A4,2X,2E12.4)

1	1-6	MATNO	ENDF/B tape material number.
2	7-22	MATHOL	Material name.
3	25-36	TEMTUR	$\leq$ 0 = no effect T = temperature (in °Kelvin) for doppler broadening of resonance cross sections
4	37-48	SIGP	Non-resonance isotopes potential scattering cross sections in barns per absorber atom (see part B)

Card No. 3 (12I6)

Item	Cols.	Name	Description
1	1-6	LINK1A	0 = no effect. 1 = process pointwise cross sections. (must be 1 if LINK2A = 1)
2	7-12	LINK1B	0 = no effect. 1 = calculate group cross sections.
3	13-18	LINK2A	0 = no effect. 1 = calculate pointwise kerma factors. (must be 1 if LINK2B = 1)
4	19-24	LINK2B	0 = no effect. 1 = calculate group kerma factors.
5	25-30	IPRT1A	0 = no effect. 1 = print pointwise cross sections.
6	31-36	IPRT1B	0 = no effect. 1 = print group cross sections.
7	37-42	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 factors on tape.
8	43-48	IPRT2B	0 = no effect. 1 = print group kerma factors.
9	49-54	IPUN1A	0 = no effect. 1 = punch pointwise cross sections except inelastic levels. 2 = punch pointwise cross sections for all reactions.

Item	Cols.	Name	Description
10	55-60	IPUN1B	0 = no effect. 1 = punch group reaction cross sections.
11	61-66	IPUN2A	0 = no effect. 1 = punch pointwise kerma factors by reaction (and total). 2 = punch pointwise total kerma factor.
12	67-72	IPUN2B	0 = no effect. 1 = punch group kerma factors.

Card No. 4 (12I6)

1	1-6	IRESON	0 = no effect. 1 = calculate resonance cross sections if resonance parameters are present. 2 = read resonance cross sections from tape (logical unit 8).
2	7-12	KEY	1 = process all reactions on ENDF/B tape for that material. 2 = process only the reactions specified on Card No. 11.
3	13-18	IWXS	1 = flat weighting for group cross sections. 2 = 1/E weighting for group cross sections.
4	19-24	IWKF	1 = flat weighting for group kerma factors. 2 = 1/E weighting for group kerma factors. 3 = weighting is input 4 = weighting is input * 1/E

Card No. 5 (12I6)

1	1-6	INEP	1 = calculate energy point mesh. 2 = read energy points. 3 = use energy mesh from previous material.
2	7-12	NEP	number of energy points for the energy mesh. (not used if INEP = 3)
3	13-18	NRANGE	number of energy ranges with equal lethargy intervals ($\leq$ 10). (used only if INEP = 1)

Item	Cols.	Name	Description
4	19-24	NGRPS	number of energy group (<300). (not used if INEP = 3 and/or both LINK1B and LINK2B are zero).
5	25-30	IGAM	1 = GAM-II 100-group structure. 2 = input energy group structure.

Card No. 6 (12I6): This card is entered only if INEP = 1.

1	1-6	NIR(1)	number of energy points in range number 1 (see part B for detailed description).
2	7-12	NIR(2)	number of energy points in range number 2.
⋮		⋮	
NRANGE		NIR(NRANGE)	number of energy points in the last range.

Note: The user must ensure that NEP = $1+\sum_{i} NIR_i$

Card No. 7 (6E12.4)

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

1	1-12	ERB(1)	lowest energy for range number 1. (= lowest point for the energy mesh).
2	13-24	ERB(2)	lowest energy for range number 2. (= highest energy for range number 1.
3	25-36	ERB(3)	lowest energy for range number 3.
⋮		⋮	
etc.			
⋮		⋮	
NRANGE		ERB(NRANGE)	lowest energy for range number NRANGE.
NRANGE+1		ERB(NRANGE+1)	highest energy for range number NRANGE. (= highest energy point for the energy mesh).

Card No. 8 (6E12.4)

This is actually a card set and consists of the points of the energy mesh.

It is entered only if INEP = 2.

1	1-12	EP(1)	energy point number 1. (lowest energy).

Item	Cols.	Name	Description
2	13-24	EP(2)	energy point number 2.
3	25-36	EP(3)	energy point number 3.
⋮		⋮	
etc. using NEP/6 cards			
⋮		⋮	
NEP		EP(NEP)	energy point number NEP. (highest energy).

Card No. 9 (6E12.4)

This is a card set and is entered only if a) INEP = 1 or 2, and b) LINK1B and/or LINK2B is 1. It consists of the desired energy group structure.

1	1-12	EGRPB(1)	energy group breakpoint number 1. (lowest energy).
2	13-24	EGRPB(2)	energy group breakpoint number 2.
⋮		⋮	
etc. using (NGRPS + 1)/6 cards			
⋮		⋮	
NGRPS		EGRPB(NGRPS)	energy group breakpoint number NGRPS.
NGRPS+1		EGRPB(NGRPS+1)	energy group breakpoint number NGRPS+1 (highest energy).

Card No. 10 (E12.4,4A4)

1	1-12	CONVF	conversion factor to convert kerma factors from electron volt•barn/atom to any other desired units.
2	13-28	UNTHOL	maximum of 16 alphanumeric characters describing the units of kerma factors after CONVF is used.

Card No. 11 (12I6)

This can be one or two cards and is entered only if KEY = 2 and consists of the number of reactions and the MACK number for each reaction desired (see detailed input Part B).

Item	Cols.	Name	Description
1	1-6	NREAC	number of reactions to be processed for this material.
2	7-12	IR(1)	MACK number for the first reaction.
3	13-18	IR(2)	MACK number for the second reaction.
⋮		⋮	
NREAC+1		IR(NREAC)	MACK number for the last reaction.

Card No. 12 (6E12.4)

This is actually three cards and they are always required. The decay energies for the various reactions are entered on these three cards in units of electron volts. Decay energies for the reactions which are not required are not used and the corresponding fields can be left blank.

Item	Cols.	Name	Description E decay for:	ENDF/B Reaction Number (MT)
1	1-12	DECG	(n,γ)	102
2	13-24	DECP	(n,P)	103
3	25-36	DECD	(n,d)	104
4	37-48	DECT	(n,t)	105
5	49-60	DECHE3	(n,He3)	106
6	61-72	DECA	(n,α)	107
7	1-12	DEC2A	(n,2α)	108
8	13-24	DEC3A	(n,3α)	109
9	25-36	DECN2N	(n,2n)	16
10	37-48	DNPA	(n,n')α	22
11	49-60	DNP3A	(n,n')3α	23
12	61-72	D2NA	(n,2n)α	24
13	1-12	DNPP	(n,n')P	28

Card(s) No. 13

This set of cards is required if IWKF = 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 frm low to high energy.

Card 13.1 (2I11)

Item	Cols.	Name	Description
1	1-11	N1	Number of interpolation ranges.
2	12-22	N2	Number of weighting function points.

Card 13.2 (6I11)

1	1-11	NBT(1)	Last point number in first interpolation range.
2	12-22	JNT(1)	Interpolation scheme for first range.
3	23-33	NBT(2)	Last point number in 2nd interpolation range.
4	34-44	JNT(2)	Interpolation scheme for second range.
⋮		⋮	
etc.			
2*N1-1		NBT(N1)	Last point number in the N1 interpolation range.
2*N1		JNT(N1)	Interpolation scheme for the N1 range.

Card 13.3 (6E11.4)

1	1-11	X(1)	First energy point ($\leq$ lowest energy of the energy point mesh).
2	12-22	Y(1)	Weight at this energy.
etc. (using N2/3 cards)			
2*N2-1		X(N2)	Last energy point ($\geq$ highest energy in the energy point mesh.
2*N2		Y(N2)	Weight at this energy.

B. Detailed Input Data Notes

Each case consists of one card (Card No. 0) followed by one or more data sets. Each data set is an input for one material and consists of the required cards from Cards No. 1 through No. 13.

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

Card No. 0

An incorrect IDTAP will result in an error message but will not hinder the execution.

1 - Card No. 1

SIGP (σ_p) is the potential scattering cross section in barns per atom of the resonance nuclide for the other nuclides which are admixed with the resonance nuclide. σ_p is used in the unresolved resonance calculation as explained in Appendix B. Using an equivalence theorem this parameter can be used to mock cell leakages by including an effective escape cross section value.

In the narrow resonance approximation, $\overline{\sigma_p}$, the effective scattering cross section per absorber atom is given by

$$\overline{\sigma_p} = \sigma_{p_a} + \frac{1}{N_a\left(\frac{\overline{1}_o}{1-C}\right)} + \sigma_m$$

where

σ_{p_a} = potential scattering of the absorber atom

σ_m = the sum of the scattering cross sections per absorber atom for all moderators in the absorber lump.

N_a = lump absorber atom density

$\overline{l_o}$ = radius or thickness of the absorber lump.

C = Dancoff pin shadowing factor[25].

The quantity SIGP is given then by

$$SIGP = \frac{1}{N_a\left(\frac{\overline{l_o}}{1-C}\right)} + \sigma_m$$

The case of infinite dilution is obtained by inputting large SIGP (e.g. 10^8).

2 - Card No. 3 (LINKS and Output Options)

The calculations performed in the MACK code is divided into four links (in addition to the resonance link described on the next card). These links are:

1. Pointwise cross sections (LINK1A),
2. Group reaction cross sections (LINK1B),
3. Pointwise kerma factors (LINK2A),
4. Group kerma factors (LINK2B).

LINK1A must be 1 if LINK1B is 1. Also, LINK2A must be 1 if LINK2B is 1. If kerma factors are desired (i.e. LINK2A = 1) LINK1A must be 1.

LINK1B calculates the reaction (e.g. (n,α)) cross section by group. It does not calculate the transfer cross section between groups.

IPRT2A

This is an option for printout and writing an output tape for pointwise kerma factors.

IPRT2A = 0, no print and no output tape for pointwise kerma factors.

IPRT2A = 1, print pointwise kerma factors for each reaction processed.

IPRT2A = 2, pointwise kerma factors for each reaction processed are written on a (BCD) card image tape (no print).

IPRT2A = 3, both 1 and 2 (print and write tape for pointwise kerma factors by reaction).

IPRT2A = 4, only total kerma factor to be printed and written on tape.

For all output options (print, punch, tape) if the output by reaction option is specified it implies that the sum of the pointwise kerma factors (total kerma factor) is included in the output.

If LINK2B = 1, the group kerma factors are calculated for the seven reaction types in table 1 section 2 and the total kerma factor. As noted in table 1, each type is a sum over all reactions that belong to that type.

3 - Card No. 4

IRESON

As mentioned earlier, if the resonance parameters are present in ENDF/B file 2 for the 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. Of these four cross sections, only elastic scattering and radiative capture are important for the MACK code.

If IRESON = 1, these calculations will be performed in the MACK code if resonance parameters are given in file 2.

IRESON = 0 hinders the execution of such calculations. The energy range for the resonance region extends generally from 1 eV to less than 500 KeV. If the resonance energy region is outside the energy range specified for pointwise cross section and kerma calculation, IRESON should be set equal to zero. If elastic scattering and radiative capture are not among the desired reactions, IRESON should be zero.

If IRESON = 2, the code will skip the resonance calculation part and expects the resonance cross section on the tape (logical unit 8). The tape may be the output saved from a previous MACK run for the same material or produced by any other means.

This option has two merits. First, the resonance calculations need not be repeated if it is desired to process the same material several times. The other merit is that it allows the user to use the resonance cross sections generated by any other processing code. The data expected on the resonance tape is discussed next.

If IRESON = 2, the MACK code expects a resonance cross section tape (on logical unit 8) which has two binary records. The first record is for elastic scattering and the second is for radiative capture resonance cross sections. Each record of these can be written by a FORTRAN statement of the type

```
WRITE(N)MAT,MT,L,NM,(X(K),K=L,NM)
```

where

MAT = ENDF/B material number

MT = ENDF/B reaction number

= 2 for elastic scattering

= 102 for radiative capture

L = 0

NM = size of the array X

= NEP where NEP is the number of points in the energy mesh specified on input data Card No.5.

X = "average" point resonance cross section array.

The resonance cross sections must correspond to the energy points generated or read into MACK in order of increasing energy. These resonance cross sections should not contain the background cross sections of file 3.

KEY

If KEY = 1, the code will search for all reactions of the material on ENDF/B tape which are significant for energy deposition (all reactions on table 5). If KEY = 2, only the reactions specified on card No. 11 are processed.

IWXS

If IWXS = 1, the weighting function to be used in generating the energy group cross section is 1.0. If IWXS = 2, the weighting function is 1/E.

IWKF

This option defines the weighting function to be used for generating energy group kerma factors.

IWKF equals 1 and 2 are options for flat and 1/E weighting, respectively. If IWKF = 3, the function entered on Card No. 13 (as tabulated points) is used as the weighting function. If IWKF = 4, the weighting function used is the input function (on Card No. 13) multiplied by 1/E. Other built in weighting functions can be easily added to the program if desired.

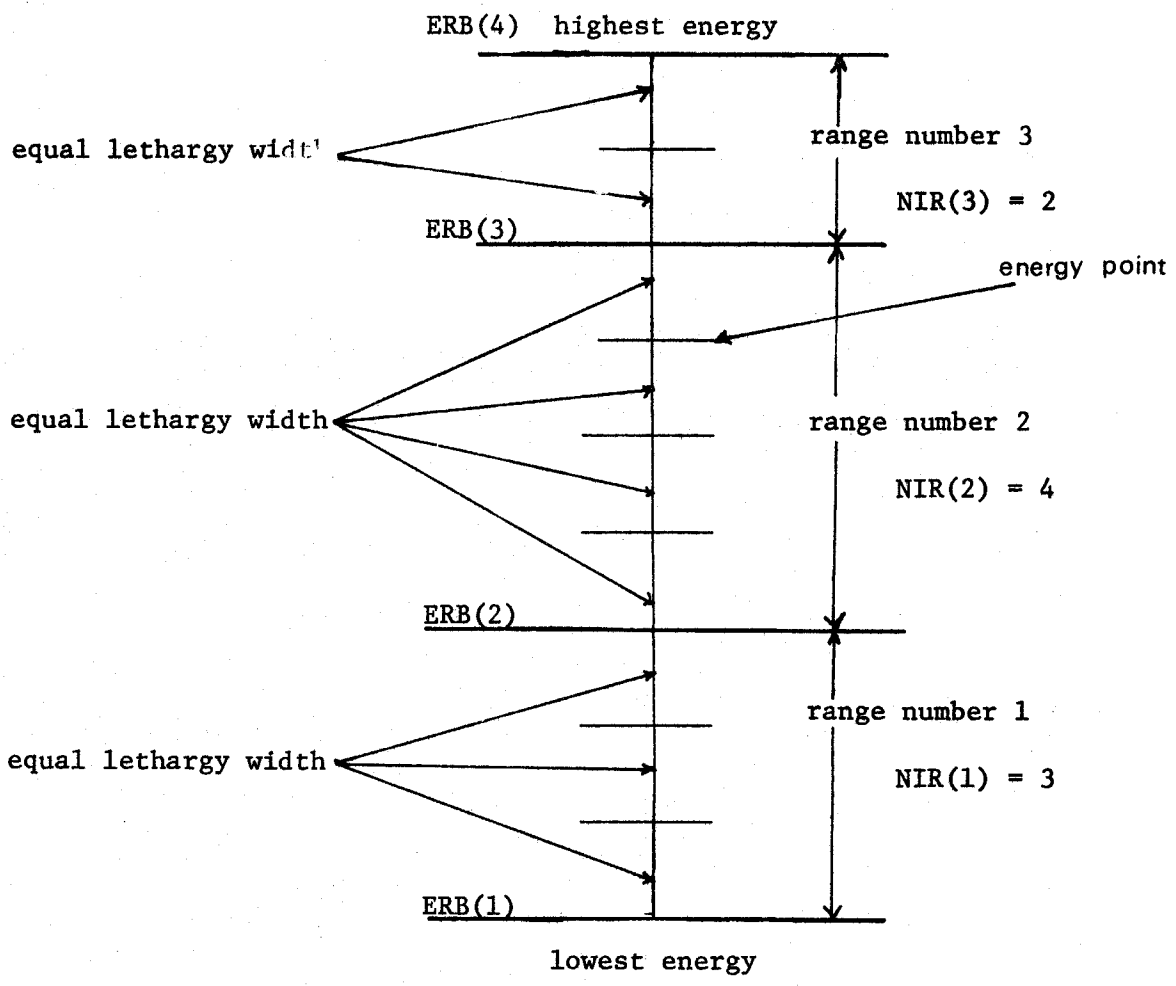
4 - Cards No. 5 through No. 9

This set of cards flexibly specifies the desired energy mesh and group structure. It should be noted that all energies in the input are always entered in units of electron volts and in the order of increasing energy.

If INEP = 3, the energy mesh and group structure, if any, are used from the previous material and Cards 6 through 9 should not be entered.

If INEP = 2, Cards No. 6 and No. 7 should not be entered and the energy mesh is entered on the next card (No. 8) in the order of increasing energy (FORMAT (6E12.4)). 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 No. 6 and No. 7 are needed in this case and they specify the characteristics of the energy mesh. The total energy range is divided in the code into a number of energy ranges given by the entry NRANGE. The energy breakpoints for these ranges are entered in the array ERB which has NRANGE+1 entries. Each range, i, is divided into 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 further expalins these parameters.



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

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

NRANGE=number of energy ranges = 3

NEP = number of energy points in the mesh

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

$$= 10$$

Figure 2. Schematic diagram for the relation between the energy mesh parameters.

The energy group structure is entered on Card Set No. 9 and is entered only if all of the following conditions are met:

1. INEP = 1 or 2,
2. LINK1B and/or LINK2B = 1,
3. IGAM is not 1.

The energy group breakpoints if entered, are in the 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 is 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 15 MeV (20 MeV for some materials).

If IGAM = 1, the GAM-II one-hundred energy group structure is used.

5 - Card No. 10

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 volts·barn/atom. The conversion factor, CONVF, entered on Card No. 10 is used by the code to convert the kerma factors into any other desired units. CONVF can also be used to obtain the macroscopic kerma factors for the material by including the nuclide density x 10^{-24} in it. CONVF should be entered as 1.0 if no conversion is desired.

6 - Card No. 11

If KEY = 2 on Card No. 4, the MACK numbers for the required reactions are entered on Card No. 11 in any desired order. The MACK numbers for all reactions are given in table 5 and the corresponding ENDF/B MT numbers are also designated. If any of the MACK numbers 6 through 10 ((n,p), (n,d), (n,t),(n,He3) and (n,α)) are specified, the corresponding reations in the 700's series (reaction cross section to the various levels, e.g. (n,Po), (n,P_1)) are also processed. Incidentally, the MACK numbers are used in the input only and converted in the code into the corresponding MT numbers which are used throughout the program.

7 - Card No. 12 (E_{decay})

As mentioned in the theory section (section II), a nuclear reaction is followed, in some instances, by radioactive decay of the activated residual nucleas. The energy, E_{decay}, of charged particles emitted in such decay must be added to the energy release by the primary recoil. Methods for calculating E_{decay} were given in section II. Values of E_{decay} were calculated using these methods for all reactions in a limited number of materials and are distributed with the code.

E_{decay} for all the reactions are entered on Card No. 12 (three cards) in units of electron volts. In general, E_{decay} is non-zero only for four or five reactions. E_{decay}'s for reactions not present on ENDF/B tape for the material (or not required by input) are not used and the corresponding fields can be left blank.

TABLE 5

Reaction MACK Numbers
(for use on input data Card No. 11)

MACK No.	Reaction Type	MT
1	Elastic	2
2	Inelastic Level	51-90
3	(n,2n)	16
4	Not used	-
5	(n,γ)	102
6*	(n,P)	103
7*	(n,d)	104
8*	(n,t)	105
9*	(n,He3)	106
10*	(n,α)	107
11	(n,2α)	108
12	Not used	-
13	(n,3α)	109
14	(n,n'α)	22
15	(n,n'3α)	23
16	(n,n')P	28
17	Inelastic Scattering to Continuum	91
18	(n,2n)α	24

* The corresponding reactions (partial reaction cross sections to the various levels) in the 700's series are also processed.

E_{decay} can be energy dependent for a mixture of isotopes as explained earlier. However, this energy dependence was found to be generally less important than the energy dependence of the reaction Q-value (assumed energy-independent in present ENDF/B format). Therefore, the energy dependence of E_{decay} was ignored in the present version of the code. This will be revised if the ENDF/B format changes.

If it is desired to calculate the kerma factors without the contribution of radioactive decay, E_{decay} should be entered as zero (or blank) for all reactions. The kerma factor for a reaction, at a particular energy, E, from radioactive decay contribution alone is merely E_{decay} times the reaction cross section at E. For energy-independent (or nearly so) E_{decay}, group cross sections can be used. Hence, the calculation of radioactive decay kerma factors can be easily performed (the reactions cross sections can be punched from a MACK run).

8 - Card No. 13 (weighting function)

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

The weighting function is entered as tabulated points in pairs 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. 13.2 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.

9 - Multiple Cases

Any number of materials on the ENDF/B tape can be processed in a single run in the order in which they appear on the tape (increasing order of material number). If INEP is entered as 3 for a material, the energy point mesh and the energy group structure, if any, of the preceeding material are used.

10 - Logical Tape Numbers

The logical tape numbers used as variables throughout the program are given their numeric values in the main program. The tape assignments required by MACK are as follows:

Logical Tape	
2	scratch-always required
3	output pointwise kerma factors - required only if IPRT2A (on input data Card No. 3) is > 1
5	standard input
6	standard output
7	punch (should be changed to 1 for UNIVAC-1108)
8	resonance cross section tape (required if IRESON is not zero)
10	ENDF/B library tape

Note: If IRESON = 1 (on input data Card No. 4), unit 8 is used as a scratch tape for resonance calculations. At the end of the resonance calculations, the resonance cross sections are written on logical unit 8 for later use in the program. If IRESON = 2, the code reads the input resonance cross section from logical unit 8 . In both cases, the resonance cross section tape is saved if not more than one resonance nuclide is processed in the same run.

C. MACK Output Description

C. 1 Description of Printed Output

The first output section consists of a message about the ENDF/B tape ID compared with input data tape ID (IDTAP) and a brief edit of the input data. The code checks some of the input data (e.g. the energy group structure is checked to see if it is in the order of increasing energy) and if any error is found self-explanatory messages are printed and the run is terminated.

The following section is a short printout of the descriptive section of ENDF/B file 1 of the material and it provides a brief documentation of how the data for the nuclide were evaluated. The pointwise energy mesh (read from input or calculated) and the corresponding lethargy mesh are printed next.

For resonance nuclides, the calculation in the resonance link follows. The first part of this section is a list of the resonance energies and parameters in the resolved region, doppler broadening temperature and the number of resolved resonance points calculated in the code. The second part is a printout of the pointwise resonance cross sections calculated for the resolved region followed by those of the unresolved region. The last part of that section is the "point average" cross sections (for elastic scattering and radiative capture) at the points of the required energy mesh (kerma energy mesh).

The cross sections by reaction follow. The cross sections 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 = 50-91). A list of ENDF/B reaction numbers, MT, is given at the end of this section. The MT reaction Q-value is also printed. If LR is not zero, Q1 is the Q-value for the n,n' part of the reaction and Q2 is the Q-value corresponding to the combined reaction LR. 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. The pointwise cross sections printed in this section are obtained from

ENDF/B file 3. For resonance nuclides, the final cross sections are printed with the pointwise kerma factors. The group cross sections printed (and punched) include the resonance contribution, if any, and are in order of increasing group number (order of decreasing energy). A message is printed in this section about each reaction searched for and not found on the ENDF/B tape.

The following section is the pointwise kerma factors by reaction. 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 print for the pointwise kerma factor of a reaction is a tabulation by energy point of the cross section, energy release per reaction (includes radioactive decay contribution, E_{decay} of the reaction), and the kerma factor. The pointwise kerma factors by reaction are printed only if IPRT2A is equal to 1 or 3.

The following section is always printed and consists of the kerma factors classified into the seven kerma reaction types given in table 1 (section II) in addition to the the total pointwise kerma factor. The kerma factor for each of these seven types is a sum over the kerma factors of the corresponding MT numbers designated in table 1.

If both LINK2B and IPRT2B equal 1, the last section is a printout of energy group kerma factors for each of the seven kerma reaction types. The total group kerma factors are also printed by group. The group kerma factors are not printed for any kerma reaction type (e.g. (n,n') charged particles) if it is zero for all energy groups.

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	°Kelvin
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 UNTHOL using the conversion factor CONVF specified on input data Card No. 10.

C. 2 Description of Punched Output

If IPUN2A is not zero, the first section of punch is the energy point mesh in increasing order of energy. The pointwise and group cross sections are punched followed next by pointwise and group kerma factors. The punched card output for each section is determined from the appropriate punch options on input data Card No. 3. The information punched for each section is discussed below.

Pointwise Cross Sections [IPUN1A > o]

1. Title card (input data card)
2. Reaction title card
3. Array of pointwise cross sections by energy point in the order of increasing energy.

Group Cross Sections [IPUN1B = 1]

1. Title card
2. Reaction title card
3. A card with 54* in the first three columns.
4. Array of group cross sections by energy group in the order of increasing group number (decreasing energy).
5. A card with T in the third column.

Pointwise Kerma Factors [IPUN2A > 0]

1. ID card
2. Array of pointwise kerma factors by energy point in order of increasing energy.

The ID card consists of the following information [FORMAT(A4,I4,4A4,2I4,5A4,I3,5A4)]

Cols.	Description
1-4	the four characters ****
5-8	ENDF/B material number (MATNO)
9-24	alphanumeric description of the material (MATHOL)
25-28	number of energy points (NEP)
29-32	ENDF/B kerma factor reaction number (MT + 300)
33-52	alphanumeric equivalent of the MT reaction
53-55	ENDF/B LR flag
56-75	alphanumeric equivalent of the reaction corresponding to LR

The ID card for the total kerma factor has the same format with a reaction number of 301 in columns 29-32, the characters TOTAL KERMA FACTOR in columns 33-52 and columns 53-75 are blank.

The kerma factors reaction numbers were chosen according to ENDF/B specifications[10] of adding 300 to the corresponding reaction (MT) number. For example, for elastic scattering (MT = 2), the reaction number for the kerma factor for elastic scattering is 302.

The energy mesh is punched with an ID of the same format with a dummy reaction number of -1.

Group Kerma Factors [IPUN2B = 1]

Group kerma factors are punched for the seven kerma reaction types (see table 1) and for the total (sum over all reactions). The format of the punched cards is the same as for group cross sections.

All the arrays are punched in ANISN[11] format with the repeat (R) option.

C. 3 Description of Output on Logical Unit 3

If IPRT2A = 2 or 3, the pointwise kerma factors by reaction and the total kerma factors are written on tape (logical unit 3) in BCD mode. If IPRT2A = 4, only total kerma factors are written on the tape. In both cases, the kerma factors are preceded by the energy mesh.

The pointwise kerma factors are written in the same format as the punched output explained above. The tape is not rewound between nuclides and hence, the pointwise kerma factors can be written on the tape for all or some of the materials in the run. An end of file mark is written on the tape only after all materials in the run have been completed.

Definition of Reaction Types

Reaction types are identified in ENDF/B by an integer, MT. A list of the allowed reaction types are given below.[10] These numbers are used in MACK.

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)
16*	(n,2n) cross section
17	(n,3n) cross section
18	Total fission cross section (sum of MT=19, 20, 21, plus any undefined part)
19	(n,f) cross section
20	(n,n'f) cross section
21	(n,2nf) cross section
22*	(n,n')α cross section
23*	(n,n')3α cross section
24*	(n,2n)α cross section
25	(n3n)α cross section
26	(to be assigned)
27	(no longer used)
28*	(n,n')p cross section
29	Scattering (sum of MT=2 and 4) (Note: MT=29 no longer used)

MT	Description
30-50	(to be assigned)
51*	(n,n') to the 1st excited state
52*	(n,n') to the 2nd excited state
⋮	
90*	(n,n') to the 40th excited state
91*	(n,n') to the continuum
92-100	(to be assigned)
101	Parasitic absorption (redundant, sum of MT=102, 103, 104, 105, 106, 107, 108, 109)
102*	(n,γ) radiative capture cross section
103*	(n,p) cross section
104*	(n,d) cross section
105*	(n,t) cross section
106*	(n,He^3) cross section
107*	(n,α) cross section
108*	$(n,2\alpha)$ cross section
109*	$(n,3\alpha)$ cross section
110-150	(to be assigned)
151	General designation for resonance information
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

MT	Description
254-300	(to be assigned)
301-450	Energy release rate parameters, $\overline{E^*\sigma}$, for total and partial cross sections. Subtract 300 from this number to obtain the specific reaction type identification. For example, MT=302=(300+2) denotes elastic scattering.
451	Heading or title information (only fiven in File 1)
452	$\bar{\upsilon}$, average total (prompt plus delayed) number of neutrons released per fission event
453	Radioactive decay chain data
454	Fission product yield data
455	Delayed neutrons from fission
456-699	(to be assigned)
700*	(n,p_0) cross section (cross section for leaving the residual nucleas in the grounded state)
701*	(n,p_1) cross section for 1^{st} excited state
702*	(n,p_2) " " " 2^{nd} " "
703*	(n,p_3) " " " 3^{rd} " "
704*	(n,p_4) " " " 4^{th} " "
⋮	
718*	(n,p_{18}) " " " 18^{th} " "
719*	(n,p_c) " " " continuum
720*	(n,d_0) cross section for ground state
721*	(n,d_1) cross section for 1^{st} excited state
722*	(n,d_2) " " " 2^{nd} " "
⋮	
738*	(n,d_{18}) " " " 18^{th} " "
739	(n,d_c) " " " continuum
740*	(n,t_0) cross section for ground state

MT	Description
741*	(n,t_1) cross section for 1st excited state
742*	(n,t_2) " " " 2nd " "
⋮	
758*	(n,t_{18}) " " " 18th " "
759*	(n,t_c) " " " continuum
760*	(n,He_0^3) cross section for ground state
761*	(n,He_1^3) cross section for 1st excited state
⋮	
779*	(n,He_c^3) " " " continuum
780*	(n,α_0) cross section for ground state
781*	(n,α_1) cross section for 1st excited state
⋮	
799*	(n,α_c) " " " continuum
800-999	(to be assigned)

---

* These reactions are processed by MACK.

V. MISCELLANEOUS INFORMATION

The purpose of this section is to provide a programmer with useful information about some of the internal details of the MACK program.

Since $\overline{E_{Hi}(E) * \sigma(E)}$ is not generally equal to $\overline{E_{Hi}(E)} * \overline{\sigma(E)}$ the code is programmed to calculate $E_{Hi} * \sigma_i(E)$ at any desired energy mesh specified by input. If the group kerma factors are desired, they are processed in the program at any desired group structure from the pointwise kerma factors. It should be obvious that the accuracy of group kerma factors increases as the number of energy points (NEP) at which the pointwise kerma factors are calculated is increased.

The options for calculating group cross sections for selected or all reactions in addition to the group kerma factors provide a rapid and economical way of obtaining a complete "activity" set for calculation of reaction rates of interest, neutron heating and dose rates in any nuclear system.

The MACK source program consists of approximately 5700 cards in 69 subprograms listed with their external references at the end of this section. The program is entirely in standard FORTRAN IV and should be machine-independent. The FORTRAN functions ERF, ERFC and AUXERF may be removed from the program if routines for calculating the error and complementary error functions are available in the software of the particular installation. Statements for obtaining and printing the CPU time may be added in subroutine CLOCK. A large number of comments are included in the various parts of the program to facilitate making any desired additions or modifications.

The flow of the calculation is shown in figure 3 and a suggested overlay structure is given in figure 4. The MAIN program calls

subroutine CONTRL which controls the flow of the calculation according to the input options selected. At this time, segment 1 will be brought in. In segment 1, the input is read, the energy mesh is generated, ENDF/B tape is positioned to the desired material, and file 1 is read and printed out. The test for the values of the variables LRP and IRESON is done next in subroutine CONTRL. If both are 1, subroutine RESONA will be called and overlay segment 2 is brought into the computer. Subroutine RESONA is the administrative routine for resonance calculations. Subroutine TMFRES reads file 2 data. The resolved and unresolved resonance calculations are executed in subroutines RESR and RESU, respectively. At the end of the resonance calculations, the resonance contribution to the cross sections at the points of the kerma energy mesh is written on a scratch device for later use.

Next, CONTRL tests the value of LINK1A. If LINK1A = 1, subroutine XSECN is called and segment 3 is brought into the computer. This is the principal subroutine for processing the smooth cross sections and the Q-values from file 3. The resonance cross sections, if any, are added to the smooth values in this link. Subroutine XSECN searches for all reactions significant for energy deposition. For each reaction, XSECN calls subroutine TMF3 for reading file 3 data and subroutine SIGPR for performing the basic processing required. In SIGPR, a test is made to see if group cross sections are requested. Subroutine CROSG is the principal routine for calculating energy group cross sections by reaction.

When flow control returns to CONTRL, the option for processing

pointwise kerma factors is investigated and if LINK2A = 1, overlay segment 4 will be brought in for this purpose. Subroutine EKERMA is the administrative routine for this calculation. For each reaction processed in segment 3, EKERMA processes the rest of the nuclear data required for energy release calculation from files 4 and 5. For each ENDF/B MT reaction number subroutine EKERMA finds out the appropriate reaction type of the seven types given in table 1. There is a subroutine with a self-explanatory name for calculating the pointwise kerma factors for each of these seven types. The radioactive decay contribution, if any, is added in these seven subroutines. In subroutines INELL and INELC (for inelastic to level and to continuum, respectively) the ENDF/B LR flag is tested and the reaction type for kerma calculation is found and the appropriate radioactive decay contribution is added. For example, if LR = 28, the type is (n,n') charged particles and the energy release from radioactive decay is calculated from E_{decay} specified in input (Card No. 12) for (n,n')p. After the calculation for all reactions are carried out, the energy group kerma factors are calculated if requested by input. Subroutine KERMAG is the principle subroutine for this calculation.

When control flow returns to subroutine CONTRL, it starts processing a new material or exits from the computer if no additional data is available.

The main arrays in the four segments use the same machine storage locations. Hence, a partial overlay is accomplished internally in the program. Because of this and the efficient equivalence of various

large arrays used within the same segment, adequate storage is available on a 65 K words machine for running problems with more than 1000 energy points. In addition, the suggested overlay structure on figure 4 saves about 9000 words. When this overlay structure is used, almost all the materials currently on ENDF/B3 including the resonance nuclides, can be run with MACK with 1500 energy points in less than 65 K words. The program has no restriction on the size of the problem provided that adequate core storage is available.

MACK uses the variable dimension technique and therefore, the array sizes are set for the particular problem only at execution time. The only exception is the size of the arrays in standard[15] COMMON/RECS/ into which the ENDF/B data records are read. In its present form, however, it accomodates all the data for all materials on the present ENDF/B.

Subroutine SIZE has the function of setting the amount of storage available to the calculation. The amount of storage is defined by the dimensions of the array D in COMMON/ZIZI/; the variable LIMIT must be set equal to this dimension. The amount of storage can be easily changed by modifying two FORTRAN statements in subroutine SIZE and recompiling. The subroutine is intentionally made simple and easy to remember. It has the following form:

```
SUBROUTINE SIZE (LIMIT)
COMMON/ZIZI/ D(25000)
LIMIT = 25000
RETURN
END
```

LIMIT must be equal to or larger than the largest of the following

a) K = 17 * NEP + 1 if LINK2A ≠ 0

or K = 12 * NEP + 1 if LINK2A = 0

b) L = 3 * MAXP + NEP + 1 if the nuclide has resonance parameters in file 2; otherwise, L = 0.

NEP is the number of points for the kerma energy mesh specified in input (see section IV) and MAXP is the number of resolved resonance points. MAXP is equal to N * M where N is the number of resolved resonances given in ENDF/B data for a resonance nuclide and M is the number of energy points required per resonance. M is selected in MACK as follows. If the number of resolved resonances, N, is less than or equal to 130, the energy mesh for resolved resonance calculations is generated with 50 energy points per resonance; i.e. M = 50. For N greater than 130, M is set to 24.

After reading the input, the program calculates the amount of storage required for the problem and if the value of LIMIT is not adequate, the code prints out an error message and terminates the case.

The segments in the overlay structure given in figure 4 can be further broken down into a larger number of levels if desired. The external references given in the list of the subroutines at the end of this section is useful in this regard.

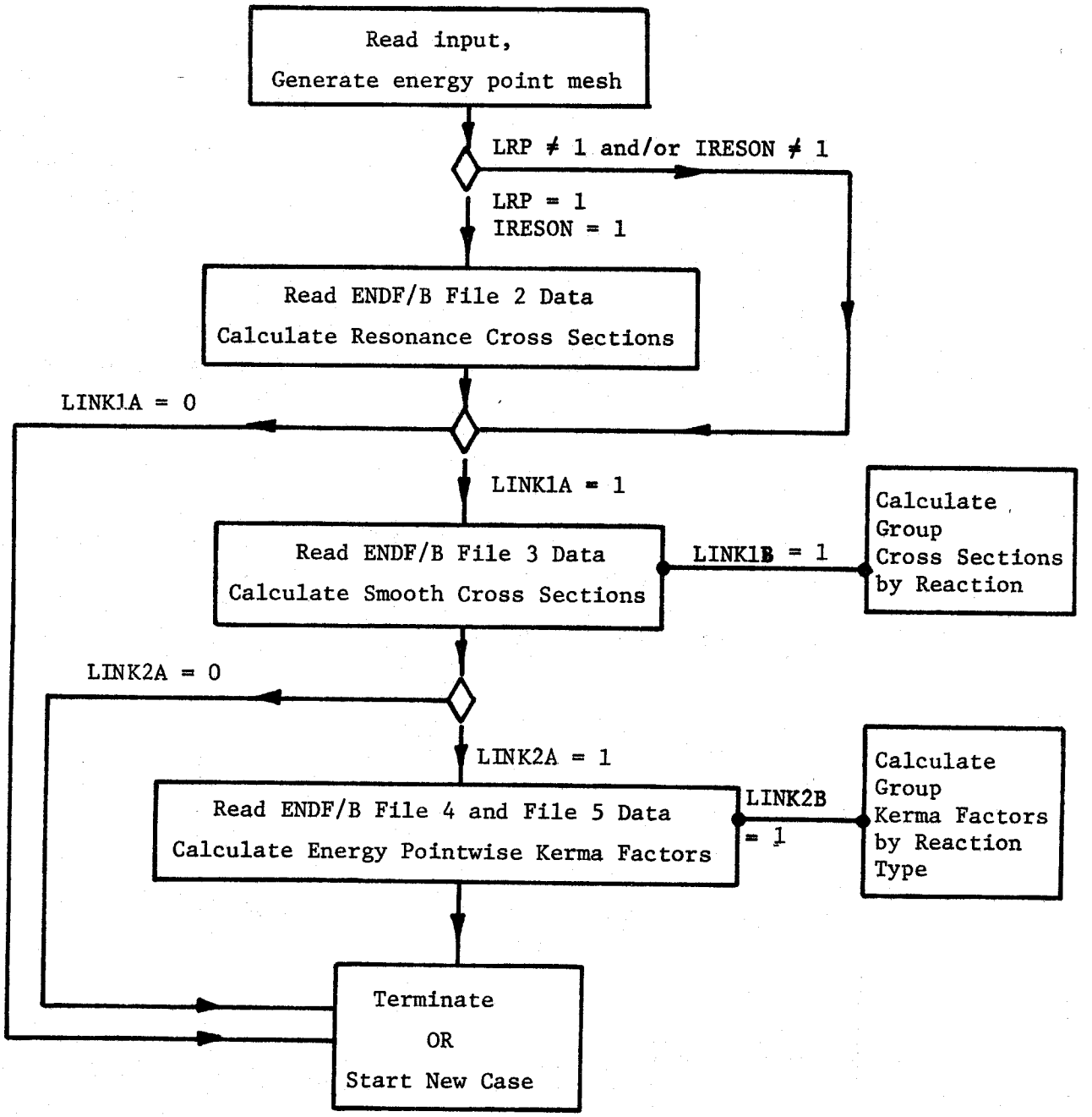
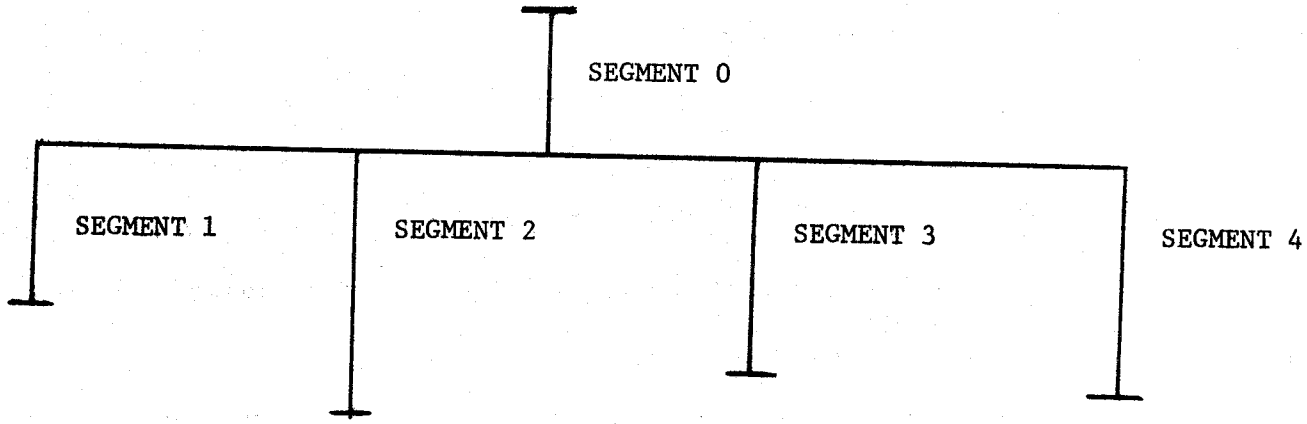


Figure 3. Calculational Flow Chart for MACK

Figure 4. Overlay Structure for MACK



SEGMENT 0					
MAIN	TERP2	RITE	WT1E	TPOS	ERF
CONTRL	SCRAT	PUNSH	ZEROA	TAB1	ERFC
SIZE	FINDI	DTFPUN	MOVE	TAB2	AUXERF
MTID	FINDIM	GRATE	CONT	ERROR	TERPO
TERP1	FLTFX	ECSI	LIST	CLOCK	
SEGMENT 1					
TRID	TMF1	IN5	START	EPOINT	
TMAT	SKPFIL	HOLL			
SEGMENT 2					
RESONA	TMFRES	RESR	RESU	RXSECT	
MESH	FILL	BROAD			
SEGMENT 3					
XSECN	GRPRES	TMF3	SIGPR		
SIGC	CROSG	WEIT			
SEGMENT 4					
EKERMA	COST	ELAST	INELL	RN2N	INELC
EBAR	GAMMA	CHARG	NPCHG	KERMAG	HANDY
TITLE	WRIT	TMF4	CMLAB	TMF5	

List of Subroutines

1. MAIN - main program

   Calls: TRID, CONTRL, SIZE

2. CONTRL - administrative routine to various links of the program.

   Calls: START, IN5, TMAT, TMF1, EPOINT, RESONA, XSECN, WEIT, EKERMA

3. START - initializes some varialbes in named common.

4. IN5 - reads and writes out input data.

5. EPOINT - generates energy mesh according to input options.

   Calls: PUNSH

6. TRID - reads ENDF/B tape ID record

   Calls: CONT

7. TMAT - positions ENDF/B tape to a desired material number.

   Calls: CONT, HOLL

8. TMF1 - reads ENDF/B file 1 data

   Calls: HOLL, CONT, LIST, TAB1, SKPFIL

9. RESONA - administrative routine for resonance calculations

   Calls: TMFRES, RESR, RESU, RXSECT

10. TMFRES - reads ENDF/B file 2 (resonance parameters data).

    Calls: CONT, LIST

11. RESR - resolved resonance calculations.

    Calls: MESH, CLOCK, BROAD

12. MESH - constructs energy mesh for resolved resonance

    Calls: FILL

13. FILL - auxiliary routine for MESH

14. BROAD - Doppler broadening treatment.

    Calls: ERFC

15. RESU - unresolved resonance treatment

    Calls: TERPO

16. RXSECT - Calculates "average" point resonance cross section

    Calls: GRATE, SCRAT, FINDI, FINDIM

17. XSECN - administrative routine for smooth cross section calculations.

    Calls: GRPRES, TMF3, SIGPR, MOVE, SIGC, SCRAT, ZEROA

18. SIGPR - calculates and stores smooth cross sections for one reaction.

    Calls: TERP2, MTID, CROSG, FINDI, SCRAT, PUNSH, FINDIM, RITE

19. CROSG - calculates energy group cross sections

20. GRPRES - prepares resonance contribution to group cross sections.

    Calls: SCRAT, FINDI, GRATE, WT1E

21. SIGC - saves repeated CALLs in XSECN.

    Calls: SCRAT

22, 23. ZEROA, MOVE - zero an array and move information from one place to another.

24. EKERMA - administrative routine for energy release calculations

    Calls: SCRAT, COST, ELAST, INELL, EBAR, RN2N, INELC, GAMMA, CHARG, NPCHG, PUNSH, KERMAG

25. ELAST - kerma calculation for elastic scattering.

    Calls: TITLE, WRIT

26. INELL - kerma calculation for inelastic level.

    Calls: TITLE, FINDIM, WRIT

27. INELC - kerma calculation for inelastic to continuum

    Calls: HANDY, WRIT, TITLE

28. CHARG - kerma calculation for charged particle reactions

    Calls: SCRAT, ZEROA, WRIT, TITLE

29. NPCHG - kerma calculation for (n,n', charged particles) reactions.

    Calls: HANDY, WRIT, TITLE

30. GAMMA - kerma calculation for radiative capture

    Calls: HANDY, WRIT, TITLE

31. RN2N - kerma calculation for (n,2n) reactions

    Calls: HANDY, WRIT, TITLE

32. HANDY - performs operations required by kerma subroutines

33. KERMAG - calculates energy group kerma factors

    Calls: GRATE, WT1E, RITE, PUNSH, FINDI

34. WT1E - integrates a function weighted by 1/E

    Calls: TERPO

35. RITE - writes desired portions of arrays

36. TITLE- stores the alphanumeric equivalent of a reaction type number

    Calls: MTID

37. WRIT - output routine for energy point kerma factors

    Calls: PUNSH

38. ERROR - prints error message

39. COST - retrieves angular distribution data and calculates the average of the cosine of the scattering angle.

    Calls: TMF4, CMLAB, TERP2, GRATE, FINDI, RITE

40. CMLAB - transforms legendre coefficients from laboratory to center-of-mass system.

41. EBAR - calculates the average energy of a secondary neutron.

    Calls: TMF5, TERPO, TAB1, GRATE, RITE, ERF

42. TERP1 - interpolates one point.

    Calls: ERROR

43. TERP2 - forms a new table by interpolation.

    Calls: ERROR, TERP1

44. TERPO - interpolates a point from TAB1 record.

45. HOLL - reads Hollerith material description.

    Calls: LIST, CONT

46. TPOS - positions ENDF/B tape to desired file and reaction type number.

    Calls: CONT

47. CONT - reads control (CONT) record.

48. LIST - reads LIST record.

49. TAB1 - reads TAB1 record.

50. TAB2 - reads TAB2 record.

51. TMF3 - reads ENDF/B file 3.

    Calls: TPOS, TAB1, CONT

52. TMF4 - reads ENDF/B file 4.

    Calls: TPOS, TAB1, TAB2, CONT, LIST

53. TMF5 - reads ENDF/B file 5.

    Calls: TPOS, TAB1, TAB2, LIST

54. SKPFIL - skips the remainder of an ENDF/B file.

55. PUNSH - sets up each card written out by DTFPUN.

    Calls: DTFPUN

56. DTFPUN - punches cards or writes a card image tape in the ANISN format.

    Calls: FLTFX

57. FLTFX - converts floating point number to integer.

58. ECSI - calculates integral of y(x).

    Calls: ERROR

59. GRATE - integrates TAB1 function

    Calls: ECSI, ERROR

60. MTID - determines the alphanumeric equivalent of a reaction type number.

61. SCRAT - writes and reads a scratch binary tape.

62. FINDI - locates the lower index for the non-zero elements of an array.

63. FINDIM - locates the upper index for the non-zero elements of an array.

64. CLOCK - CPU time routine.

65. ERF (function) - computes error function.

66. ERFC (function) - computes complimentary error function.

67. AUXERF (function) - used by ERF and ERFC.

68. WEIT - reads and prepares input weighting function

    Calls: TERPZ, RITE

69. SIZE - initializes the total size of data locations.

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APPENDIX A

Sample Problems

The sample problems shown here are for illustration purposes only. The energy mesh, group structure, etc. do not necessarily represent a choice for a particular physics problem.

The sample problems do not cover all the options of the code. The output for the sample problems is not listed here but is available with the code package.

Sample Problem 1

All of the four links are requested for Lithium-7. Since MAT 1116 does not have resonance data in file 2, IRESON can be set to any value. It is suggested that IRESON be set to 1; TEMETUR and SIGP be given their appropriate values in input for all materials. If the material does have resonance parameters, these options are not used. This eliminates the need for a prior knowledge of the particular ENDF/B evaluation.

The 1/E weighting is selected for both group cross sections and kerma factors. The number of energy points is 600. The energy range is divided into three ranges with breakpoints at .02 eV, 100 eV, 1.0 MeV, and 15.0 MeV. The number of intervals of equal lethargy width are 29,300 and 270 in the 1st, 2nd and 3rd ranges, respectively. The GAM-II one-hundred group structure is selected (IGAM=1), hence card No. 9 is not entered.

CONVF is set to 1.0, hence the output kerma factors will be in the same units as those employed in the code (ELECTRON VOLT* BARN/ATOM).

The decay energies are entered as

(n,γ) E_{decay}(DECG) = 9.31 MeV

(n,d) E_{decay}(DECD) = 1.560 MeV

(n,n'P) E_{decay}(DNPP) = 1.560 MeV

and zero for all other reactions.

Sample Problem 2

In this problem, IWKF is set to 3, hence card(s) No. 13 are entered. The weighting Function is tabulated at 71 energy points. The interpolation shceme is selected as lnW(E) linear in lnE between any two points given in all the input energy range.

Sample Problem 3

This problem is for Niobium (MAT=1164). The resonance calculations are requested (IRESON=1). The temperature for Doppler broadening is 300.0°K. SIGP is entered as 1.0×10^{8} which corresponds to the infinite dilution case for the unresolved resonance calculations.

In specifying the characteristics of the energy mesh for resonance nuclides, it is important to specify a resonably large number of energy points in the resonance region.

The group structure is input (IGAM=2) from low to high in energy for 96 groups. The energy group structure should be within the energy range of the energy point mesh but does not need to cover all the energy range.

All decay energies are entered as zero, hence, no contribution to kerma factors from radioactive decay is calculated.

```
   0      2                                                                    CARD 0
          ****  MACK SAMPLE PROBLEM 1 LITHIUM-7 MAT1116    ****               CARD 1
1116 LITHIUM-7                                                                CARD 2
   1      1      1      1      1      1      1      1      0      1      2     1CARD 3
   1      1      2      2                                                     CARD 4
   1    600      3    100      1                                             CARD 5
  29    300    270                                                           CARD 6
0.02              100.0       1.0 +06     15.0  +6                          CARD 7
1.0          FV*RARN/ATOM                                                     CARD10
  9.310+06  0.0            1.560 +06                                         CARD12.1
0.0                                                                           CARD12.2
  1.560+06                                                                    CARD12.3
```

```
    0      2                                                                  CARD 0
*** MACK SAMPLE PROBLEM 2 VANADIUM MAT 1017  ***************************CARD 1
 1017 VANADIUM1017                                                          CARD 2
    1      1      1      1      1      1      1      1      0      1      2      1CARD 3
    1      1      2      3                                                   CARD 4
    1    800      4    100      1                                           CARD 5
   30    320    249    200                                                  CARD 6
 .01           50.0          5.0       +5     1.0  +07     1.5  +07         CARD 7
 1.602   -19 WATT*BARN/ATOM                                                 CARD 10
 1.070   +06 0.9340   +06                                      0.210  +06CARD12.1
 0.0                                                                        CARD12.2
 0.0                                                                        CARD12.3
          1          71                                                     CARD13.1
         71           5                                                     CARD13.2
 .1000E-03  .1000E+05  .5000E+07  .2000E-06  .7000E+07  .1429E-06          CD13.3 1
 .8000E+07  .1250E-06  .9000E+07  .1111E-06  .1000E+08  .1000E-06
 .1050E+08  .9524E-07  .1100E+08  .9091E-07  .1150E+08  .8696E-07
 .1180E+08  .8475E-07  .1200E+08  .8333E-07  .1205E+08  .8299E-07
 .1210E+08  .8265E-07  .1215E+08  .8231E-07  .1220E+08  .8197E-07
 .1225E+08  .8164E-07  .1230E+08  .8131E-07  .1235E+08  .8100E-07
 .1240E+08  .8069E-07  .1245E+08  .8041E-07  .1250E+08  .8015E-07
 .1255E+08  .7995E-07  .1260E+08  .7984E-07  .1265E+08  .7988E-07
 .1270E+08  .8014E-07  .1275E+08  .8078E-07  .1280E+08  .8200E-07
 .1285E+08  .8413E-07  .1290E+08  .8764E-07  .1295E+08  .9321E-07
 .1300E+08  .1018E-06  .1305E+08  .1148E-06  .1310E+08  .1341E-06
 .1315E+08  .1620E-06  .1320E+08  .2018E-06  .1325E+08  .2571E-06
 .1330E+08  .3326E-06  .1335E+08  .4334E-06  .1340E+08  .5647E-06
 .1345E+08  .7316E-06  .1350E+08  .9383E-06  .1355E+08  .1187E-05
 .1360E+08  .1477E-05  .1365E+08  .1804E-05  .1370E+08  .2160E-05
 .1375E+08  .2531E-05  .1380E+08  .2901E-05  .1385E+08  .3250E-05
 .1390E+08  .3555E-05  .1395E+08  .3797E-05  .1400E+08  .3959E-05
 .1405E+08  .4027E-05  .1410E+08  .3926E-05  .1415E+08  .3801E-05
 .1420E+08  .3589E-05  .1425E+08  .3306E-05  .1430E+08  .2972E-05
 .1435E+08  .2608E-05  .1440E+08  .2234E-05  .1445E+08  .1870E-05
 .1450E+08  .1530E-05  .1455E+08  .1224E-05  .1460E+08  .9587E-06
 .1465E+08  .7351E-06  .1470E+08  .5524E-06  .1475E+08  .4072E-06
 .1480E+08  .2945E-06  .1485E+08  .2093E-06  .1490E+08  .1461E-06
 .1495E+08  .1004E-06  .1500E+08  .6786E-07                              CD13.324
```

```
   0      2                                                                  CARD 0
 ******** MACK SAMPLE PROBLEM 3 NIOBIUM (WITH RESONANCE PARAMETERS)
1164 NIOBIUM                 300.0          1.0  +08                        CARD 2
   1      1      1      1      1      1      3      1      0      0      1     1CARD 3
   1      1      2      1                                                    CARD 4
   1   1000      3     96      2                                            CARD 5
  39    500    460                                                          CARD 6
 .02           10.0          5.0     +05     1.5 +07                       CARD 7
.3              .4             .55            .70           .85          1.2 CARDS 9
  .1445+01      .1855+01       .2385+01       .3059+01      .3928+01     .5043+01CARDS 9
  .6476+01      .8315+01       .1068+02       .1371+02      .1760+02     .2260+02
  .2902+02      .3727+02       .4785+02       .6144+02      .7889+02     .1013+03
  .1301+03      .1670+03       .2144+03       .2754+03      .3536+03     .4573+03
  .5829+03      .7485+03       .9611+03       .1234+04      .1585+04     .2035+04
  .2613+04      .3355+04       .4307+04       .5531+04      .7102+04     .9119+04
  .1171+05      .1503+05       .1930+05       .2479+05      .3183+05     .4087+05
  .5247+05      .6738+05       .8652+05       .1111+06      .1228+06     .1357+06
  .1500+06      .1657+06       .1832+06       .2024+06      .2237+06     .2472+06
  .2732+06      .3020+06       .3337+06       .3688+06      .4076+06     .4505+06
  .4979+06      .5502+06       .6081+06       .6721+06      .7427+06     .8208+06
  .9072+06      .1003+07       .1108+07       .1225+07      .1353+07     .1496+07
  .1653+07      .1827+07       .2019+07       .2231+07      .2466+07     .2725+07
  .3012+07      .3329+07       .3679+07       .4066+07      .4493+07     .4966+07
 .550   +07     .6065+07       .6703+07       .7408+07      .8187+07 0.900   +07CARDS 9
  .1000+08                                                                 CARDS 9
 1.0          EV*BARN/ATOM                                                 CARD10
0.0                                                                        CARD12.1
0.0                                                                        CARD12.2
0.0                                                                        CARD12.3
```

```
   0     2
 MACK SAMPLE PROBLEM 4 LITHIUM-7 - (SELECTION OF REACTIONS) ----------CARD 1
1116 LITHIUM-7                                                        CARD 2
   1     1     1     1     1     1     1     1     0     1     2     1CARD 3
   1     2     2     2                                               CARD 4
   1   600     3   100     1                                         CARD 5
  29   300   270                                                     CARD 6
0.02            100.0       1.0 +06    15.0  +6                     CARD 7
1.0         EV*BARN/ATOM                                            CARD10
   5     9     7     5    18    17                                   CARD 11
  9.310+06  0.0           1.560 +06                                 CARD12.1
0.0                                                                 CARD12.2
  1.560+06                                                          CARD12.3
```

APPENDIX B

Resonance Region Treatment

The resonance treatment in MACK for both the resolved and unresolved region is summarized below.

B. 1 Resolved Resonance Treatment

The resolved resonance parameters given in single-level Breit-Wigner (SLBW) or multi-level Breit-Wigner (MLBW) representations are processed in MACK. The treatment is equivalent to the method described in APPENDIX D of ref. 10.

The SLBW formulae, written in the laboratory system for all ℓ-values and without Doppler broadening are[10](for a particular isotope):

1. Elastic Scattering Cross Section

$$\sigma_{n,n}(E) = \sum_{\ell=0}^{NLS} \sigma^{\ell}_{n,n}(E),$$

where $\sigma^{\ell}_{n,n}(E) = (2\ell+1)\frac{4\pi}{k^2} \sin^2\phi_{\ell}$

$$+ \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma^2_{nr}\cos 2\phi_{\ell} - 2\Gamma_{nr}(\Gamma_{\gamma r} + \Gamma_{fr}) \sin^2\phi_{\ell} + 2(E-E'_r)\Gamma_{nr}\sin 2\phi_{\ell}}{(E-E'_r)^2 + \frac{1}{4}\Gamma^2_r}$$

2. Radiative Capture Cross Section

$$\sigma_{n,\gamma}(E) = \sum_{\ell=0}^{NLS} \sigma^{\ell}_{n,\gamma}(E)$$

where

$$\sigma_{n,\gamma}^{\ell}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{\gamma r}}{(E-E_r')^2 + \frac{1}{4}\Gamma_r^2} .$$

3. Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{\ell=0}^{NLS} \sigma_{n,f}^{\ell}(E) ,$$

where

$$\sigma_{n,f}^{\ell}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{fr}}{(E-E_r')^2 + \frac{1}{4}\Gamma_r^2} ,$$

where

$$g_J = \frac{2J+1}{2(2I+1)}$$

I is the spin of the target nucleas and J is the spin of the compound nucleus for the resonance state.

I = SPI, as given in File 2 data for each isotope

The summation on ℓ extends over all ℓ-states described. There will be NLS terms in the summation.

NLS is given in File 2 for each isotope

The summation on J extends over all possible J-states for a particular ℓ-state. NR_J is the number of resonance for a given pair of ℓ and J values.

$$NRS = \sum_{J} NR_J$$

NRS is given in File 2 for each ℓ-value

$\Gamma_{nr}(|E_r|) = GN_r$ is the neutron width, for the r^{th} resonance for a particular value of ℓ, evaluated at the resonance energy E_r. For bound levels, the absolute value $|E_r|$ is used.

$$\Gamma_{nr} = \frac{P_\ell(E)\ \Gamma_{nr}(|E_r|)}{P_\ell(|E_r|)}$$

$\Gamma_r = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr}$ is the total width.

The following quantities are given in File 2 for each resonance:

E_r = ER, the resonance energy

J = AJ, the spin of the resonance state

$\Gamma_{nr}(|E_r|)$ = GN, the neutron width

$\Gamma_{\gamma r}$ = GG, the radiation width

Γ_{fr} = GF, the fission width

$$E_r' = E_r + \frac{S_\ell(|E_r|) - S_\ell(E)}{2P_\ell(|E_r|)}\ \Gamma_{nr}(|E_r|)$$

$$k = 2.196771\ \frac{AWRI}{AWRI + 1.0}\ \times 10^{-3}\ \sqrt{E}\ ,$$

where k is the neutron wave number and AWRI is the ratio of the mass of the particular isotope to that of the neutron.

AWRI given in File 2 data for each isotope

E is the incident neutron energy (Laboratory system);

S_ℓ is the shaft factor,

$$S_0 = 0$$

$$S_1 = -\frac{1}{1 + \rho^2}$$

$$S_2 = -\frac{18 + 3\rho^2}{9 + 3\rho^2 + \rho^4}$$

P_ℓ is the penetration factor,

$$P_0 = \rho$$

$$P_1 = \frac{\rho^3}{1 + \rho^2}$$

$$P_2 = \frac{\rho^5}{9 + 3\rho^2 + \rho^4}$$

where $\rho = ka$ and "a" is the channel radius (in units of 10^{-12} cm) and is defined as

$$a = [1.23\ (AWRI)^{1/3} + 0.8] \times 10^{-1}\ ;$$

ϕ_ℓ is the phase shift,

$$\phi_0 = \hat{\rho}$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho}$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\frac{3\hat{\rho}}{3-\hat{\rho}^2}\ ,$$

where $\hat{\rho} = k\hat{a}$ and $\hat{a}$ is the effective scattering radius.

$\hat{a}$ = AP, as given in File 2 data

Multilevel Breit-Wigner Formula:

The equations are exactly the same as above, except that a level-level interference term is included in the equation for elastic scattering:

$$\frac{\pi}{k^2} \sum_J g_J \sum_{r=2}^{NR_J} \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left[(E-E'_r)(E-E'_s) + \frac{1}{4}\Gamma_r\Gamma_s\right]}{\left[(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2\right]\left[(E-E'_s)^2 + \frac{1}{4}\Gamma_s^2\right]}\ .$$

Subroutine RESR calculates the capture, scattering (and fission) cross sections in the resolved resonance region. The total cross section is obtained by summing the partial cross sections. The energy mesh to be used for the resolved resonance calculation is generated in subroutine MESH. The resonance energy, Er, and the total width,

Γr, are used in setting up the energy mesh to insure an adequate number of points near the resonance energy, Er.

An option is available to get Doppler broadened cross sections at an arbitrary input temperature. Subroutine BROAD uses numerical quadrature of the ordinarty ψ and χ functions to calculate Doppler broadened cross sections (at an arbitrary temperature specified by input option) from tabulated values of the unbroadened cross sections[19].

Unresolved Resonance Treatment

In the region of unresolved resonances, the average resonance parameters are spedified in ENDF/B in three formats:

1. LFW = 0 (fission widths not given)
   LRF = 1 (all parameters are energy-independent)

2. LFW = 1 (fission widths given)
   LRF = 1 (only fission widths are energy- dependent; the other parameters are energy-independent)

3. LFW = 0 or 1
   LRF = 2 (all parameters are energy-dependent)

The program permits all three formats. Calculations are done for S-, P-, and d- wave neutrons and include a summation over spin states (S) in each case. The treatment follows that of MC^2 [20] and ETOX [21].

The unresolved resonance calculations are carried out in subroutine RESU. The capture, fission and scattering cross sections are calculated at 2o1 energy points (equally spaced in lethargy) in the unresolved resonance region. A brief discussion is given next.

In the unresolved resonance region, only the average resonance parameters can be deduced. Therefore, the calculation of an average

cross section requires a knowledge of the distribution of the resonance parameters about their average value. There is, at present, no quantitative theory that can be relied upon to predict such distributions. However, Wigner, Porter and Thomas[24] using a combination of qualitative theoretical considerations with measurements in the resolved range suggested the forms of these distributions. The spacing, D, between the energy levels in a given sequence in the compound nucleus is represented by the Wigner distribution

$$P(Z) = \frac{\pi}{2} Z \, e^{-\frac{1}{4}\pi Z^2} \qquad (3.1)$$

with $Z = D/\bar{D}$

where $\bar{D}$ is the average spacing in the sequence. The distribution for partial widths of resonances is represented by a "chi-square" probability distribution with n degrees of freedom

$$P_n(r) = \frac{n}{2\Gamma(\frac{1}{2}n)} \left(\frac{nr}{2} \right)^{\frac{1}{2}n-1} e^{\frac{-nr}{2}} \qquad (3.2)$$

where $r = \dfrac{\Gamma^\circ_x}{\bar{\Gamma}^\circ_x}$

Γ°_x = reduced partial width for a given type

$\Gamma(\frac{1}{2}n)$ = gamma function of $\frac{1}{2}n$

It was found that neutron width can generally be represented with n = 1, fission width with n = 2 and radiation width with a larger n. The number of degrees of freedom, n, is specified in ENDF/B for each process.

The cross section in the unresolved resonance region is usually calculated as point average cross section over an energy interval ΔE. The energy interval must be large enough to contain

many resonances and so small that the average resonance parameters will not change much within it. The expected number of resonances within the interval ΔE will then be $\Delta E/\bar{D}$. The point average cross section at energy E* for process c in material m is given by[26]

$$\overline{\sigma_c(E^*)} = \frac{\frac{1}{\Delta E}\int_{E_1}^{E_2} \frac{\sigma_c^m(E)}{\sigma_t(E)}\,dE}{\frac{1}{\Delta E}\int_{E_1}^{E_2} \frac{1}{\sigma_t(E)}\,dE} \qquad (3.3)$$

where $\sigma_t(E)$ is the total cross section per absorber m atom and its reciprocal represents the weighting function. Eq. 3.3 can be rewritten as

$$\overline{\sigma_c(E^*)} = \frac{\frac{1}{\Delta E}\int_{E_1}^{E_2} \frac{\sum_s \sum_i \sigma_{c_i}^{m\,s}(E)}{\sum_s \sum_i \sigma_{r_i}^{s}(E) + \sigma_p}\,dE}{\frac{1}{\Delta E}\int_{E_1}^{E_2} \frac{dE}{\sum_s \sum_i \sigma_{r_i}^{s}(E) + \sigma_p}} \qquad (3.4)$$

In Eq. 3.4, the total cross section was broken into a resonant part, $\sigma_r(E)$, and the remainder which is denoted by σ_p. For the case of a mixture, $\sigma_t(E)$ should include the contribution of all other isotopes present. MACK is not programmed to process mixtures. However, σ_p is read in the input and can be used to account, to some extent, for other isotopes present in a mixture other than the resonance nuclide m. A large σ_p (e.g. 10^6) corresponds to the infinite dilution case. The sum in the

numerator of the upper integral in Eq. 3.4 ranges only over the sequences of isotope m; the other sums range over all nuclides in the mixture.

In Eq. 3.4, s represents a sequence of resonances with the same angular momentum and channel spin and the i's are the resonances in that sequence. When overlap effects between different resonances of the same sequence and overlap between more than two sequences are ignored Eq. 3.4 can be written as[26]

$$\sigma_c^m(E^*) = \frac{\sum_s^m \sum_i \frac{1}{\Delta E} \int_{E_1}^{E_2} \frac{\sigma_{c_i}^s}{\sigma_{r_i}^s + \sigma_p} \left[1 - \sum_{s' \neq s} \sum_{i'} \frac{\sigma_{r_{i'}}^{s'}}{\sigma_{r_{i'}}^{s'} + \sigma_p} \right] dE}{\frac{1}{\sigma_p} \left\{ 1 - \sum_s \sum_i \frac{1}{\Delta E} \int_{E_1}^{E_2} \frac{\sigma_{r_i}^s}{\sigma_{r_i}^{s'} + \sigma_p} \left[1 - \sum_{s'=s} \sum_{i'} \frac{\sigma_{r_{i'}}^{s'}}{\sigma_{r_{i'}}^{s'} + \sigma_p} \right] dE \right\}} \tag{3.5}$$

Since the sequences are uncorrelated, the second sequence sums in Eq. 3.4 can be integrated over the probability of finding resonance i' of s' within ΔE at a separation δE from resonance i of S[26]. With the assumption that the narrow resonance approximation is valid, the integration limits can be replaced by $-\infty$ and $+\infty$ since the contribution from resonances outside ΔE is small. Since we assumed that ΔE is large enough to contain many resonances, the summation over i can be replaced with an integration of the chi-squared probability distribution with n degrees of freedom given in Eq. 3.2. Carrying out the indicated operations on Eq. 3.5 the following expression is obtained[21]

$$\overline{\sigma_c(E^*)} = \frac{\overline{\sigma_p} \sum_{s}^{m} a_x^s \left[1 - \sum_{s' \neq s} b^{s'}\right]}{1 - \sum_{s} b^s \left[1 - \sum_{s' \neq s} b^{s'}\right]} \qquad (3.6)$$

where

$$a_x^s = \frac{1}{\langle D^s \rangle} \int_0^\infty P_n(r) \Gamma_c^s \; J(\xi^s, \beta^s) dr$$

$$b^s = \frac{1}{\langle D^s \rangle} \int_0^\infty P_n(r) \Gamma^s \; J(\xi^s, \beta^s) dr$$

$$J(\xi^s, \beta^s) = \int_0^\infty \frac{\psi^s}{\psi^s + \beta^s} \, dx$$

ψ^s is the usual ψ-function

$\xi = \Gamma/\Delta$ where Δ is the Doppler width

Γ = the average total width

$\beta^s = \overline{\sigma_p}/\sigma_o^s$ where σ_o is the peak cross section and is given by

$$\sigma_o = \frac{2.6037 \times 10^6}{E} \; g_J \; \Gamma_n \left[\frac{A + 1.0}{A}\right]^2$$

g_J = the statistical spin factor = $\frac{1}{2} \; \frac{2J + 1}{2I + 1}$

J = total angular momentum of the compound nucleas

I = the ground state spin of the target nucleas

$$x = \frac{2(E - E_o)}{\Gamma}$$

$P_n(r)$ and r are given in Eq. 3.2.

For fissile materials, an integration over the chi-squared distribution for the fission widths is included.

For sufficiently large values of β (infinite dilution), the J-function can be approximated as

$$J(\xi,\beta) \simeq J_o = \frac{\pi}{2\sqrt{\beta+\beta^2}}$$

This approximation is used in the code. The validity of this approximation is insured by inputting large SIGP which corresponds to the infinite dilution case.

The integrations over the Porter-Thomas (chi-squared) distribution of the resonance partial widths are carried out using

$$\int_o^\infty f(x)\ P_n(x)dx = \frac{1}{N}\sum_{i=1}^{N} f(xi)$$

with the x_i's properly selected as described in ref. 20 and 21. N is taken as 10 for neutron-width and 5 for fission-width distributions. Tables 3 and 4 list the x_i values which are used in the code.

TABLE 3

Used for Integration of Neutron-width Distributions with One or Two Degrees of Freedom

Index, i	Degrees of Freedom, n		Index, i	Degrees of Freedom, n	
	1	2		1	2
1	0.00525430	0.0517550	6	0.574320	0.800477
2	0.0371740	0.163089	7	0.879486	1.05263
3	0.103133	0.288398	8	1.33502	1.39297
4	0.207850	0.431720	9	2.10558	1.91582
5	0.359875	0.599144	10	4.39230	3.30400

TABLE 4

Values of x_i Used for Integration of Fission-width Distributions with One, Two, Three, or Four Degrees of Freedom

Index, i	Degrees of Freedom, k			
	1	2	3	4
1	0.0212093	0.107400	0.189269	0.254966
2	0.155477	0.360070	0.476304	0.549072
3	0.467072	0.699863	0.793185	0.842565
4	1.10710	1.22312	1.23576	1.23075
5	3.24914	2.60955	2.30575	2.12265

APPENDIX C

Average β-particle Kinetic Energy

On the following pages, the average β-particle kinetic energy is tabulated as a function of the atomic number, Z, and the endpoint energy, E_o, of the β-spectrum. Each table is for a particular atomic number, Z, for β^- or β^+. The first column of each table is the endpoint energy for the β-spectrum and the second column is the corresponding average kinetic energy. The ratio of the average to the endpoint kinetic energy is given in column 3.

These tables were computed using the Fermi-theory of β-decay as explained in section II and they are in excellent agreement with experiment.

BETA DECAY

Z= 0

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0033	33.4321
.02	.0067	33.5295
.03	.0101	33.6259
.04	.0135	33.7211
.05	.0169	33.8154
.06	.0203	33.9087
.07	.0238	34.0009
.08	.0273	34.0922
.09	.0308	34.1825
.10	.0343	34.2718
.20	.0702	35.1158
.30	.1076	35.8783
.40	.1463	36.5701
.50	.1860	37.2003
.60	.2267	37.7764
.70	.2681	38.3048
.80	.3103	38.7912
.90	.3532.	39.2401
1.00	.3966	39.6556
1.50	.6201	41.3399
2.00	.8512	42.5619
2.50	1.0872	43.3867
3.00	1.3263	44.2100
3.50	1.5677	44.7904
4.00	1.8106	45.2662
4.50	2.0548	45.6632
5.00	2.3000	45.9993
5.50	2.5458	46.2874
6.00	2.7922	46.5371
6.50	3.0391	46.7554
7.00	3.2864	46.9481
7.50	3.5339	47.1193
8.00	3.7818	47.2723
8.50	4.0299	47.4100
9.00	4.2781	47.5346
9.50	4.5265	47.6477
10.00	4.7751	47.7510
11.00	5.2726	47.9325
12.00	5.7704	48.0871
13.00	6.2686	48.2202
14.00	6.7670	48.3360
15.00	7.2657	48.4377
16.00	7.7644	48.5277
17.00	8.2633	48.6079
18.00	8.7624	48.5798

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 1

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0031	31.3900
.02	.0064	32.0662
.03	.0097	32.4291
.04	.0131	32.6863
.05	.0164	32.8925
.06	.0198	33.0691
.07	.0233	33.2263
.08	.0267	33.3706
.09	.0302	33.5048
.10	.0336	33.6316
.20	.0694	34.3824
.30	.1066	35.5402
.40	.1452	36.2904
.50	.1848	36.9613
.60	.2254	37.5679
.70	.2668	38.1204
.80	.3090	38.6262
.90	.3518	39.0911
1.00	.3952	39.5203
1.50	.6187	41.2497
2.00	.8499	42.4969
2.50	1.0859	43.4376
3.00	1.3251	44.1715
3.50	1.5666	44.7592
4.00	1.8096	45.2406
4.50	2.0539	45.6417
5.00	2.2990	45.9810
5.50	2.5449	46.2717
6.00	2.7914	46.5234
6.50	3.0383	46.7436
7.00	3.2856	46.9375
7.50	3.5332	47.1100
8.00	3.7811	47.2639
8.50	4.0292	47.4025
9.00	4.2775	47.5277
9.50	4.5259	47.6414
10.00	4.7745	47.7452
11.00	5.2720	47.9277
12.00	5.7699	48.0829
13.00	6.2682	48.2166
14.00	6.7666	48.3328
15.00	7.2652	48.4349
16.00	7.7640	48.5252
17.00	8.2630	48.6057
18.00	8.7620	48.6778

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 1

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0035	35.4743
.02	.0070	34.9797
.03	.0104	34.3094
.04	.0139	34.7441
.05	.0174	34.7279
.06	.0208	34.7390
.07	.0243	34.7671
.08	.0278	34.8055
.09	.0314	34.8525
.10	.0349	34.9050
.20	.0711	35.5456
.30	.1086	36.2142
.40	.1474	36.8484
.50	.1872	37.4383
.60	.2279	37.9841
.70	.2694	38.4888
.80	.3116	38.9559
.90	.3545	39.3888
1.00	.3979	39.7908
1.50	.6215	41.4301
2.00	.8525	42.6269
2.50	1.0884	43.5360
3.00	1.3275	44.2487
3.50	1.5688	44.8216
4.00	1.8117	45.2920
4.50	2.0558	45.6847
5.00	2.3009	46.0176
5.50	2.5467	46.3031
6.00	2.7930	46.5508
6.50	3.0399	46.7675
7.00	3.2871	46.9587
7.50	3.5347	47.1288
8.00	3.7825	47.2809

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 10

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.4983
.02	.0052	26.1592
.03	.0080	26.7371
.04	.0109	27.2362
.05	.0138	27.6735
.06	.0168	28.0636
.07	.0199	28.4154
.08	.0230	28.7374
.09	.0261	29.0338
.10	.0293	29.3098
.20	.0628	31.3860
.30	.0985	32.8434
.40	.1360	34.0025
.50	.1749	34.9760
.60	.2149	35.8187
.70	.2559	36.5615
.80	.2978	37.2244
.90	.3404	37.8219
1.00	.3836	38.3638
1.50	.6071	40.4751
2.00	.8388	41.9386
2.50	1.0754	43.0154
3.00	1.3152	43.8409
3.50	1.5573	44.4936
4.00	1.8009	45.0220
4.50	2.0456	45.4587
5.00	2.2913	45.8257
5.50	2.5376	46.1382
6.00	2.7845	46.4075
6.50	3.0317	46.6419
7.00	3.2793	46.8477
7.50	3.5272	47.0299
8.00	3.7754	47.1923
8.50	4.0237	47.3380
9.00	4.2722	47.4693
9.50	4.5209	47.5883
10.00	4.7697	47.6967
11.00	5.2675	47.8867
12.00	5.7657	48.0479
13.00	6.2642	48.1863
14.00	6.7629	48.3064
15.00	7.2617	48.4116
16.00	7.7607	48.5045
17.00	8.2598	48.5872
18.00	8.7590	48.3612

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 10

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0049	49.4465
.02	.0091	45.6920
.03	.0132	43.8656
.04	.0171	42.7409
.05	.0210	41.9675
.06	.0248	41.4004
.07	.0287	40.9668
.08	.0325	40.6257
.09	.0363	40.3516
.10	.0401	40.1281
.20	.0784	39.1900
.30	.1173	39.1006
.40	.1570	39.2604
.50	.1976	39.5145
.60	.2388	39.8060
.70	.2808	40.1094
.80	.3233	40.4123
.90	.3664	40.7082
1.00	.4099	40.9940
1.50	.6336	42.2427
2.00	.8644	43.2182
2.50	1.0996	43.9847
3.00	1.3381	44.6047
3.50	1.5789	45.1101
4.00	1.8212	45.5304
4.50	2.0648	45.8853
5.00	2.3094	46.1886
5.50	2.5548	46.4507
6.00	2.8008	46.6794
6.50	3.0472	46.8806
7.00	3.2941	47.0590
7.50	3.5414	47.2182
8.00	3.7889	47.3612
8.50	4.0367	47.4902
9.00	4.2847	47.6073
9.50	4.5328	47.7140
10.00	4.7812	47.8116
11.00	5.2782	47.9839
12.00	5.7757	48.1311
13.00	6.2736	48.2584
14.00	6.7717	48.3694
15.00	7.2701	48.4672
16.00	7.7686	48.5539
17.00	8.2673	48.6314
18.00	8.7662	48.7010

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 20

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1657
.02	.0051	25.3900
.03	.0077	25.6466
.04	.0104	25.9124
.05	.0131	26.1780
.06	.0159	26.4395
.07	.0187	26.6940
.08	.0216	26.9417
.09	.0245	27.1817
.10	.0274	27.4144
.20	.0588	29.4115
.30	.0930	30.9874
.40	.1292	32.2956
.50	.1671	33.4136
.60	.2063	34.3904
.70	.2468	35.2518
.80	.2882	36.0221
.90	.3304	36.7144
1.00	.3734	37.3411
1.50	.5964	39.7627
2.00	.8283	41.4163
2.50	1.0654	42.6168
3.00	1.3058	43.5271

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 20

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0059	58.9259
.02	.0108	53.9321
.03	.0154	51.2723
.04	.0198	49.5358
.05	.0241	48.2860
.06	.0284	47.3325
.07	.0326	46.5763
.08	.0368	45.9597
.09	.0409	45.4462
.10	.0450	45.0122
.20	.0856	42.7803
.30	.1261	42.0172
.40	.1669	41.7363
.50	.2084	41.6712
.60	.2503	41.7165
.70	.2928	41.8224
.80	.3357	41.9626
.90	.3791	42.1213
1.00	.4229	42.2888
1.50	.6470	43.1363
2.00	.8776	43.8786
2.50	1.1124	44.4970
3.00	1.3503	45.0111

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 30

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1496
.02	.0051	25.3059
.03	.0076	25.4744
.04	.0103	25.6522
.05	.0129	25.8357
.06	.0156	26.0220
.07	.0183	26.2100
.08	.0211	26.3977
.09	.0239	26.5848
.10	.0268	26.7705
.20	.0570	28.5037
.30	.0900	30.0040
.40	.1252	31.3095
.50	.1623	32.4575
.60	.2008	33.4748
.70	.2407	34.3861
.80	.2816	35.2041
.90	.3235	35.9458
1.00	.3662	36.6186
1.50	.5884	39.2300
2.00	.8203	41.0144
2.50	1.0576	42.3049
3.00	1.2984	43.2790
3.50	1.5413	44.0381
4.00	1.7859	44.6464
4.50	2.0315	45.1439
5.00	2.2779	45.5581
5.50	2.5249	45.9080
6.00	2.7724	46.2074
6.50	3.0203	46.4664
7.00	3.2685	46.6926
7.50	3.5169	46.8919
8.00	3.7655	47.0687
8.50	4.0143	47.2266
9.00	4.2632	47.3684
9.50	4.5122	47.4966
10.00	4.7613	47.6130
11.00	5.2598	47.8160
12.00	5.7585	47.9874
13.00	6.2574	48.1340
14.00	6.7565	48.2607
15.00	7.2557	48.3714
16.00	7.7550	48.4688
17.00	8.2544	48.5553
18.00	8.7539	48.6326

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 30

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0065	65.1391
.02	.0120	59.7877
.03	.0170	56.7842
.04	.0219	54.7515
.05	.0266	53.2475
.06	.0312	52.0737
.07	.0358	51.1239
.08	.0403	50.3354
.09	.0447	49.6679
.10	.0491	49.0941
.20	.0919	45.9339
.30	.1339	44.6416
.40	.1760	44.0000
.50	.2183	43.6659
.60	.2610	43.5000
.70	.3040	43.4338
.80	.3474	43.4300
.90	.3912	43.4665
1.00	.4353	43.5308
1.50	.6601	44.0097
2.00	.8907	44.5336
2.50	1.1252	45.0083
3.00	1.3627	45.4224
3.50	1.6023	45.7804
4.00	1.8436	46.0902
4.50	2.0862	46.3600
5.00	2.3298	46.5963
5.50	2.5743	46.8048
6.00	2.8194	46.9898
6.50	3.0651	47.1550
7.00	3.3112	47.3033
7.50	3.5578	47.4371
8.00	3.8047	47.5585
8.50	4.0519	47.6690
9.00	4.2993	47.7700
9.50	4.5470	47.8627
10.00	4.7948	47.9481
11.00	5.2910	48.1000
12.00	5.7877	48.2311
13.00	6.2849	48.3453
14.00	6.7824	48.4458
15.00	7.2802	48.5348
16.00	7.7783	48.6142
17.00	8.2765	48.6854
18.00	8.7749	48.7497

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 40

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1484
.02	.0051	25.2955
.03	.0076	25.4454
.04	.0102	25.5977
.05	.0129	25.7530
.06	.0155	25.9104
.07	.0182	26.0687
.08	.0210	26.2282
.09	.0237	26.3878
.10	.0265	26.5472
.20	.0562	28.0924
.30	.0885	29.4994
.40	.1231	30.7626
.50	.1595	31.8965
.60	.1975	32.9180
.70	.2369	33.8398
.80	.2774	34.6777
.90	.3189	35.4381
1.00	.3613	36.1333
1.50	.5828	38.3528
2.00	.8144	40.7203
2.50	1.0518	42.0725
3.00	1.2928	43.0917
3.50	1.5360	43.8846
4.00	1.7807	44.5185
4.50	2.0266	45.0359
5.00	2.2733	45.4657
5.50	2.5205	45.8282
6.00	2.7683	46.1378
6.50	3.0163	46.4051
7.00	3.2647	46.6383
7.50	3.5133	46.8434
8.00	3.7620	47.0252
8.50	4.0109	47.1873
9.00	4.2600	47.3329
9.50	4.5091	47.4642
10.00	4.7583	47.5833
11.00	5.2570	47.7910
12.00	5.7559	47.9660
13.00	6.2550	48.1154
14.00	6.7542	48.2445
15.00	7.2536	48.3570
16.00	7.7530	48.4561
17.00	8.2525	48.5439
18.00	8.7520	48.6223

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 40

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0070	69.5821
.02	.0128	64.1772
.03	.0183	61.0397
.04	.0235	58.8660
.05	.0286	57.2271
.06	.0336	55.9276
.07	.0384	54.8616
.08	.0432	53.9657
.09	.0479	53.1986
.10	.0525	52.5327
.20	.0974	48.7061
.30	.1410	46.9988
.40	.1842	46.0620
.50	.2275	45.5021
.60	.2709	45.1552
.70	.3146	44.9398
.80	.3585	44.8100
.90	.4026	44.7384
1.00	.4471	44.7074
1.50	.6728	44.8545
2.00	.9035	45.1754
2.50	1.1379	45.5151
3.00	1.3750	45.8326
3.50	1.6142	46.1210
4.00	1.8551	46.3772
4.50	2.0972	46.6052
5.00	2.3404	46.8084
5.50	2.5845	46.9901
6.00	2.8292	47.1531
6.50	3.0745	47.3000
7.00	3.3203	47.4330
7.50	3.5665	47.5538
8.00	3.8131	47.6640
8.50	4.0600	47.7648
9.00	4.3072	47.8575
9.50	4.5546	47.9429
10.00	4.8022	48.0219
11.00	5.2979	48.1630
12.00	5.7943	48.2856
13.00	6.2911	48.3929
14.00	6.7883	48.4877
15.00	7.2858	48.5720
16.00	7.7836	48.6474
17.00	8.2816	48.7153
18.00	8.7798	48.7767

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 50

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1487
.02	.0051	25.2946
.03	.0076	25.4401
.04	.0102	25.5861
.05	.0129	25.7321
.06	.0155	25.8793
.07	.0182	26.0262
.08	.0209	26.1740
.09	.0237	26.3212
.10	.0265	26.4685
.20	.0558	27.9059
.30	.0877	29.2418
.40	.1219	30.4630
.50	.1579	31.5744
.60	.1955	32.5851
.70	.2345	33.5062
.80	.2748	34.3462
.90	.3160	35.1137
1.00	.3582	35.8190
1.50	.5789	38.5937
2.00	.8103	40.5128
2.50	1.0476	41.9046
3.00	1.2886	42.9547
3.50	1.5320	43.7714
4.00	1.7769	44.4236
4.50	2.0230	44.9552
5.00	2.2698	45.3964
5.50	2.5172	45.7680
6.00	2.7651	46.0851
6.50	3.0133	46.3587
7.00	3.2618	46.5974
7.50	3.5105	46.8066
8.00	3.7594	46.9920
8.50	4.0084	47.1574
9.00	4.2575	47.3057
9.50	4.5067	47.4394
10.00	4.7561	47.5606
11.00	5.2549	47.7717
12.00	5.7539	47.9495
13.00	6.2531	48.1011
14.00	6.7525	48.2319
15.00	7.2519	48.3460
16.00	7.7514	48.4463
17.00	8.2510	48.5351
18.00	8.7506	48.6144

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 50

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0073	72.9521
.02	.0135	67.6159
.03	.0193	64.4407
.04	.0249	62.2032
.05	.0302	60.4932
.06	.0355	59.1217
.07	.0406	57.9853
.08	.0456	57.0217
.09	.0506	56.1897
.10	.0555	55.4617
.20	.1023	51.1518
.30	.1474	49.1174
.40	.1918	47.9383
.50	.2359	47.1884
.60	.2801	46.6871
.70	.3244	46.3417
.80	.3688	46.1015
.90	.4134	45.9342
1.00	.4582	45.8194
1.50	.6850	45.6652
2.00	.9160	45.7989
2.50	1.1503	46.0117
3.00	1.3872	46.2393
3.50	1.6261	46.4592
4.00	1.8666	46.6639
4.50	2.1083	46.8514
5.00	2.3511	47.0222
5.50	2.5948	47.1777
6.00	2.8391	47.3189
6.50	3.0841	47.4476
7.00	3.3296	47.5653
7.50	3.5755	47.6731
8.00	3.8218	47.7721
8.50	4.0684	47.8633
9.00	4.3153	47.9475
9.50	4.5624	48.0256
10.00	4.8098	48.0980
11.00	5.3051	48.2283
12.00	5.8011	48.3421
13.00	6.2975	48.4424
14.00	6.7944	48.5313
15.00	7.2916	48.6108
16.00	7.7891	48.6821
17.00	8.2869	48.7465
18.00	8.7849	48.8050

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 60

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1486
.02	.0051	25.2942
.03	.0076	25.4390
.04	.0102	25.5833
.05	.0129	25.7273
.06	.0155	25.8704
.07	.0182	26.0137
.08	.0209	26.1561
.09	.0237	26.2982
.10	.0264	26.4403
.20	.0556	27.8203
.30	.0873	29.1103
.40	.1212	30.2997
.50	.1570	31.3906
.60	.1943	32.3883
.70	.2331	33.3035
.80	.2731	34.1404
.90	.3142	34.9096
1.00	.3562	35.6167
1.50	.5763	38.4198
2.00	.8074	40.3696
2.50	1.0447	41.7877
3.00	1.2857	42.9578

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 60

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0076	75.6131
.02	.0141	70.4004
.03	.0202	67.2364
.04	.0260	64.9766
.05	.0316	63.2314
.06	.0371	61.8191
.07	.0424	60.6398
.08	.0477	59.6327
.09	.0529	58.7579
.10	.0580	57.9878
.20	.1066	53.3214
.30	.1531	51.0268
.40	.1986	49.6475
.50	.2437	48.7368
.60	.2886	48.1020
.70	.3335	47.6443
.80	.3785	47.3071
.90	.4235	47.0551
1.00	.4687	46.8656
1.50	.6966	46.4391
2.00	.9280	46.4001
2.50	1.1624	46.4947
3.00	1.3991	46.6367

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 70

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1485
.02	.0051	25.2941
.03	.0076	25.4387
.04	.0102	25.5826
.05	.0129	25.7258
.06	.0155	25.3679
.07	.0182	26.0096
.08	.0209	26.1502
.09	.0237	26.2906
.10	.0264	26.4299
.20	.0556	27.7810
.30	.0871	29.0432
.40	.1208	30.2110
.50	.1564	31.2864
.60	.1936	32.2746
.70	.2323	33.1819
.80	.2721	34.0151
.90	.3131	34.7836
1.00	.3549	35.4898
1.50	.5746	38.3050
2.00	.8054	40.2725
2.50.	1.0427	41.7066
3.00	1.2837	42.7900

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 70

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0078	77.7761
.02	.0145	72.7120
.03	.0209	69.5859
.04	.0269	67.3280
.05	.0328	65.5690
.06	.0385	64.1351
.07	.0441	62.9302
.08	.0495	61.8955
.09	.0549	60.9920
.10	.0602	60.1928
.20	.1105	55.2595
.30	.1583	52.7548
.40	.2048	51.2084
.50	.2508	50.1605
.60	.2965	49.4105
.70	.3420	48.8542
.80	.3875	48.4313
.90	.4329	48.1042
1.00	.4785	47.8478
1.50	.7076	47.1749
2.00	.9395	46.9773
2.50	1.1741	46.9656
3.00	1.4107	47.0232

BETA(-) DECAY

AVERAGE ELECTRON KINETIC ENERGY

Z= 90

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0025	25.1487
.02	.0051	25.2944
.03	.0076	25.4390
.04	.0102	25.5827
.05	.0129	25.7251
.06	.0155	25.8671
.07	.0182	26.0077
.08	.0209	26.1479
.09	.0237	26.2867
.10	.0264	26.4245
.20	.0555	27.7546
.30	.0870	28.9920
.40	.1205	30.1374
.50	.1560	31.1946
.60	.1930	32.1689
.70	.2315	33.0660
.80	.2712	33.8943
.90	.3119	34.6566
1.00	.3536	35.3615
1.50	.5727	38.1821
2.00	.8033	40.1645
2.50	1.0404	41.6144
3.00	1.2814	42.7117

BETA(+) DECAY

AVERAGE POSITRON KINETIC ENERGY

Z= 90

E MAX. MEV	E AV. MEV	EAV / EMAX (X 100)
.01	.0081	81.0933
.02	.0153	76.3481
.03	.0220	73.3372
.04	.0284	71.1221
.05	.0347	69.3718
.06	.0408	67.9282
.07	.0467	66.7029
.08	.0525	65.5411
.09	.0582	64.7064
.10	.0639	63.8736
.20	.1172	58.5812
.30	.1673	55.7625
.40	.2158	53.9545
.50	.2634	52.6865
.60	.3105	51.7479
.70	.3572	51.0279
.80	.4037	50.4612
.90	.4501	50.0065
1.00	.4964	49.6364
1.50	.7280	48.5358
2.00	.9611	48.0571
2.50	1.1961	47.8433
3.00	1.4328	47.7588