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ABSTRACT

The MACK computer program calculates energy pointwise and multigroup nuclear response functions from basic nuclear data in ENDF/B format. The new version of the program MACK-IV, incorporates major developments and improvements aimed at maximizing the utilization of available nuclear data and ensuring energy conservation in nuclear heating calculations. A new library, MACKLIB-IV, of nuclear response functions was generated in the CTR energy group structure of 171 neutron groups and 36 gamma groups. The library was prepared using MACK-IV and ENDF/B-IV and is suitable for fusion, fusion-fission hybrids, and fission applications.

I. INTRODUCTION

A primary function of the neutronics and photonics analyses of a nuclear system is to estimate a set of nuclear response rates. The calculation of a nuclear response involves an integration over the appropriate phase space of the product of the neutron (or gamma) flux and a nuclear response function. The MACK/MACKLIB system is concerned with the computation and data management of the nuclear response functions. MACK is a computer program that calculates nuclear response functions such as neutron kerma factors, gas production, and tritium production cross sections from basic nuclear data in ENDF/B format. MACKLIB is a library of nuclear response functions in multigroup format, generated with MACK and is directly usable with most transport codes.

The MACK/MACKLIB system has evolved from a strong need in the nuclear fusion field for such a capability. The first versions of MACK[1] and MACKLIB[2] were released in 1973. These early versions have been used extensively with great success in many practical applications; the most noticeable of these is the area of the neutronics analysis for "pure" fusion reactor designs. Over the past two years, major developments have been made in the calculational algorithms and new capabilities have been added into the MACK code. The new version of the code has been released recently as MACK-IV.[3] This new version maximizes the utilization of available nuclear data and is intended to be usable in more practical applications such as fission reactors, fission-fusion hybrids in addition to pure fusion and others. A new version of MACKLIB has also been produced and released as MACKLIB-IV.[4] The library was generated with MACK-IV and the primary source of basic nuclear data was ENDF/B-IV.[5] The library includes response functions for a large number of materials and has a new versatile format. The response functions are given in a fine-energy group structure (171 for neutrons and 36 for gammas). A retrieval routine is available to prepare data from MACKLIB-IV in a broader group structure.

The purpose of this paper is to present an overview of the MACK/MACKLIB system. The most important part of the MACK program concerns the calculation of the neutron kerma factors. The basic theory and the calculational algorithms for kerma factors in MACK-IV are discussed briefly in Sec. II. Consistency in preserving the energy and the relationship between the kerma factors and gamma production cross sections are delineated in this section. The general features of MACK-IV are discussed in Sec. III. A description of the important characteristics of MACKLIB-IV is the subject of Sec. IV. A summary is given in Sec. V.

II. NUCLEAR HEATING CALCULATIONAL ALGORITHMS AND MACK-IV

Calculation of the response function for nuclear heating is the central part of the program MACK. The basic theory for these calculations is summarized in this section. The major differences in the calculational algorithms between the earlier version of MACK and the present MACK-IV are also pointed out.

The nuclear heating $H_t(\vec{r})$, at any spatial point $\vec{r}$, is the sum of the neutron heating, $H_n(\vec{r})$, and the gamma heating, $H_\gamma(\vec{r})$, where[6,7]

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

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

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

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

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

$$k_{nj}(E) = \sigma_{tj}(E)\left(E + \sum_i \frac{\sigma_{ij}}{\sigma_{tj}} Q_{ij} + \sum_{i'} \frac{\sigma_{i'j}}{\sigma_{tj}} E_{Di'j} - \sum_m \frac{\sigma_{mj}}{\sigma_{tj}} \bar{E}_{n',mj} - \frac{1}{\sigma_{tj}} S^*_{E\gamma,j}\right), \tag{4}$$

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

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

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

where σ_{pe}, σ_{ca}, and σ_{pp} are the gamma-interaction cross sections for photoelectric, compton absorption, and pair-production processes, respectively; and a_{pp} is equal to 1.02 MeV. The kerma factors are flux and density independent. The heating rate can therefore be calculated from neutron and photon transport results for any system if these factors are predetermined for all materials in the system. The evaluation of $k_{\gamma j}$ is straightforward and is normally performed by the codes which generate photon-interaction multigroup cross sections such as MUG.[8] Calculation of neutron kerma factors is complicated by the variety of reactions that a neutron can undergo, the kinematics for reactions in which more than one particle is emitted, and the demand for extensive nuclear data information.

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

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

Path II. The Gamma Production Path: In this path, $S^*_{E\gamma}$ is calculated directly from the gamma production data (files 12-15 in ENDF/B) as

$$S^*_{E\gamma}\ E_n = \int \sigma_p\left(E_n, E_\gamma\right) E_\gamma \, dE_\gamma ,$$

where $\sigma_p\ E_n, E_\gamma$ is the production cross section for a photon of energy E_γ at an incident neutron energy E_n.

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

III. GENERAL FEATURES OF MACK-IV

The purpose of this section is to briefly describe the general features of MACK-IV. A simplified flow diagram of the calculations in MACK-IV is given in Fig. 1. The program calculates pointwise and/or multigroup nuclear response functions. The pointwise energy mesh, group structure, and weighting functions can be provided by input or selected from several

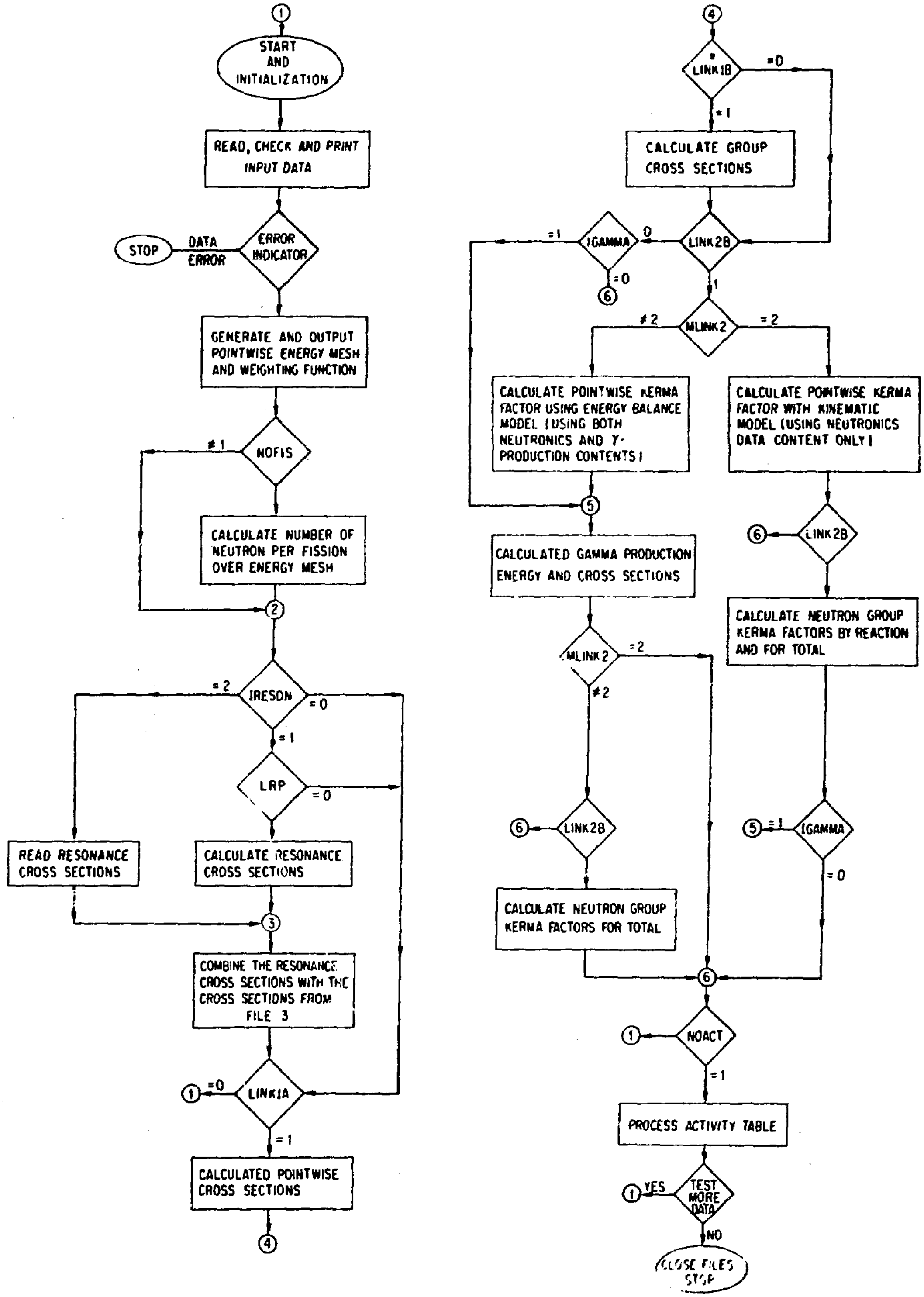

Fig. 1. A flow diagram for MACK-IV.

built-in procedures. The program has the capability to calculate the neutron cross sections in the resonance region from resonance parameters given in file 2 of ENDF/B. The program also permits reading the resonance region cross sections as input.

There are a large number of user's selected options to control the flow and methodology of computations as well as the type and format of the output. These are described in Ref. 3. All materials including fissionable isotopes can be processed by MACK-IV. Among the types of information that can be generated with MACK-IV are:

(1) Pointwise and multigroup neutron kerma factors.

(2) Pointwise and multigroup reaction cross sections.

(3) Multigroup response functions for specific nuclear processes. An example is the helium-production cross section which is calculated in MACK-IV by summing the appropriate reactions such as (n,α); $(n,n'\alpha)$ and $(n,3\alpha)$ with the multiplicities of the alpha generation accounted for.

(4) Gamma-production cross sections and the gamma-production energy matrix.

MACK-IV has a new processor that enables the user to produce the nuclear response functions for each material in the "MACK-Activity-Table" format. The format of the table is similar to that used for multigroup (transport) cross sections commonly employed in transport codes such as ANISN, DØT, and MØRSE. The data are arranged by groups (group 1, 2 . . . through group IGM) and the data for each group are given in IHM positions as illustrated in Table 1. As shown in this table, the type of information given in positions 1 through 34 is fixed. For example, the neutron kerma factor is always given in position 2 and the tritium-production cross section is given in position 7. The advantage of this format is that it provides a versatile capability for mixing the activity tables for different materials to obtain a response function table for any mixture.

One convenient way to employ the MACK-Activity-Tables is to mix them (explicitly) with the "regular transport" multigroup cross sections. The number density for each activity table should be the appropriate number density for the material multiplied by a small (e.g. 10^{-15}) fixed number, f. This multiplication factor ensures that the transport cross sections are not significantly altered. The reaction rates and other integrated responses calculated by the transport codes will be the true values multiplied by f. For this procedure to be successful the value of IHM provided as input to MACK must be equal to that employed in the regular transport multigroup cross sections (generally IHM $\geq$ IGM + 3).

The MACK-Activity-Tables can be produced in neutron-gamma-coupled format for use with coupled neutron-gamma multigroup cross sections. In this case, the gamma kerma factors have to be provided as input to MACK-IV. The data given in positions 1, 2, and 3 are such that the integrated responses for these positions are the total, neutron, and gamma heating, respectively. The atomic displacements cross sections are not calculated in MACK-IV at present but they are accepted as input to fill positions 4 and 5 of the activity table.

Table 1. MACK-Activity-Table

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

The computational time varies significantly from isotope to isotope. The CPU time is most sensitive to the requirement of cross section calculations in the resolved resonance region and Doppler broadening. Table 2 shows a sample of the CPU time on the IBM-370 Model 195 to completely process all types of data for several materials with one-thousand energy points and 171 neutron energy groups. The machine core storage requirements vary typically from ~400 to 900 k bytes on the IBM-370 Model 195 computer.

IV. MACKLIB-IV LIBRARY

A new library, MACKLIB-IV, of nuclear response functions has recently been generated. The library was prepared using MACK-IV and basic nuclear data from ENDF/B-IV. Nuclear response functions are provided in the library for all materials listed in Table 3. These materials are of great interest in fusion, fusion-fission hybrids, and fission application.

The library is in the new format of "MACK-Activity-Table" described earlier in this paper and shown in Table 1. The response functions included in the library are neutron kerma factors, gamma kerma factors, atomic displacements, gas-production and tritium-breeding functions, and all important reaction cross sections. The gamma kerma factors were generated with MUG[8] and the atomic displacements were taken from Doran's work.[9]

MACKLIB-IV employs the CTR energy group structure[10] of 171 neutron groups and 36 gamma groups. A retrieval program is included with the library to perform the following functions: (1) collapse the data into a broader group structure; (2) modify (add, delete, replace) parts of the library; (3) prepare activity tables for mixtures of materials in the library; and (4) output the data in printed, punched, and/or magnetic tape format.

As discussed in the previous section, one of the significant improvements in MACK-IV is the provision for two different calculational techniques for neutron kerma factors: (1) the nuclear kinematics path which utilizes only the neutron data files in ENDF/B; and (2) the gamma-production path which employs the gamma-production files as well as the neutron files. While the basic formalisms of the two methods are exact, the accuracy of the kerma factors calculated differs for the two methods depending on the type and accuracy of information provided in the ENDF files. The ENDF/B-IV evaluations were reviewed for each material and an appropriate calculational technique was selected to ensure the relative validity of the results.

As an example, the neutron kerma factor, k_n, for beryllium is plotted in Fig. 2 for three cases: (1) k_n based on ENDF/B-III data using the nuclear kinematics path; (2) k_n based on ENDF/B-IV data calculated with the nuclear knematics path; and (3) k_n based on ENDF/B-IV data using the gamma-production path. Comparing (1) and (2), one notes that the changes in the basic data from Version III to IV is very small. The neutron kerma factor

Table 2. Sample of CPU time (s) for MACK-IV

	Path I[a]	Path II[a]
^{6}Li	18	45
^{7}Li	18	46
Na	66	286
Cr[b]	145	237
^{238}U[b]	243	387

[a]Path I: kerma factors from nuclear kinematics.
Path II: kerma factors from gamma production path.

[b]Includes resonance calculations.

Table 3. List of Materials in MACKLIB-IV

	ENDF/B MAT No.		ENDF/B MAT No.
Hydrogen	1269	Copper	1295
Helium	1146	Niobium	1189
Lithium-6	1271	Molybdenum	1287
Lithium-7	1272	Tantalum	1285
Beryllium	1289	Tungsten-182	1128
Boron-10	1273	Tungsten-183	1129
Boron-11	1160	Tungsten-184	1130
Carbon	1274	Tungsten-186	1131
Nitrogen	1275	Lead	1288
Oxygen	1276	Thorium-232	1296
Flourine	1277	Protactinium	1297
Sodium	1156	Uranium-233	1260
Magnesium	1280	Uranium-234	1043
Aluminum	1193	Uranium-235	1261
Silicon	1194	Uranium-236	1163
Chlorine	1149	Uranium-238	1262
Potassium	1150	Neptunium	1263
Calcium	1195	Plutonium-238	1050
Titanium	1286	Plutonium-239	1264
Vanadium	1196	Plutonium-240	1265
Chromium	1191	Plutonium-241	1266
Manganese	1197	Plutonium-242	1161
Iron	1192	Americium-241	1056
Cobalt	1199	Americium-243	1057
Nickel	1190		

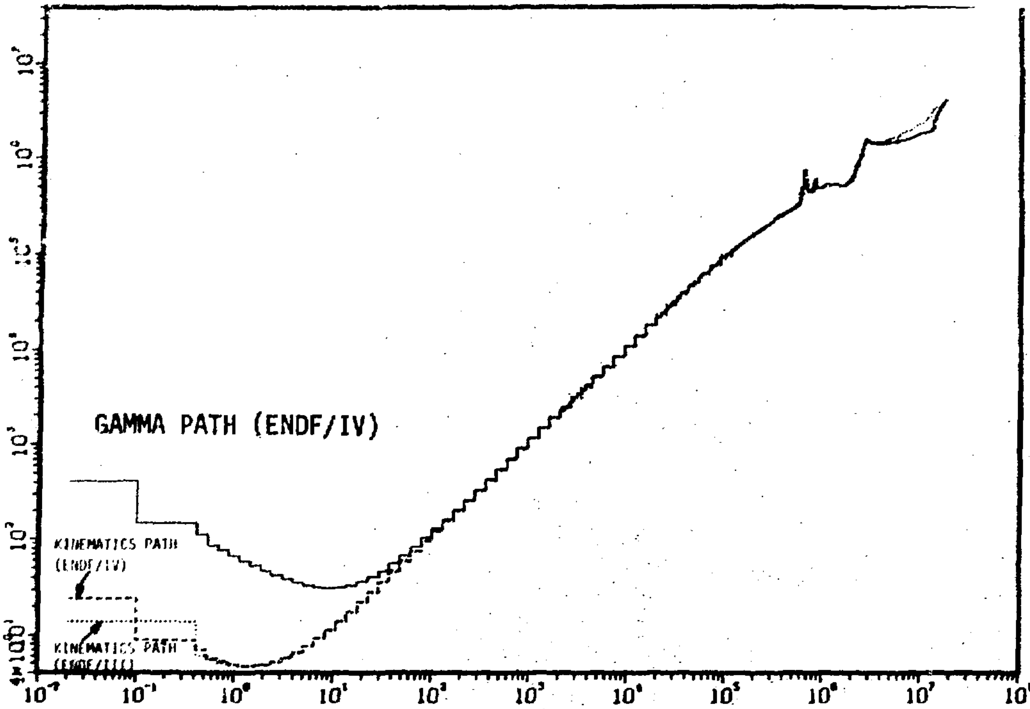

Fig. 2. Neutron kerma factors for beryllium.

calculated in Case 2 is higher than that in Case 3 at high energies (>10 MeV). The reason is that no information on the individual levels (partial level cross sections) are given in the neutron files for the (n, charged particles) reactions. In this case it is clear that the results from Case 3 are more accurate than those of Case 2 and hence the kerma factors calculated from the gamma-production path are adopted for inclusion in MACKLIB-IV.

The library also includes response functions for fissionable materials. The neutron kerma factors for ^{235}U, ^{232}Th, and ^{238}U are displayed in Fig. 3. Using the kerma factor methodology for calculation of nuclear heating in nuclear systems with fissionable materials should provide a significant improvement over the approximate methods commonly used at present. Table 4 compares the neutron kerma factors in MACKLIB-IV[4] to those in the earlier version of MACKLIB[2] for several materials. The comparison is shown for selected energy ranges where large differences occur. These differences reflect a combination of effects due to changes in basic nuclear data between Versions III and IV of ENDF/B as well as differences in calculational methods.

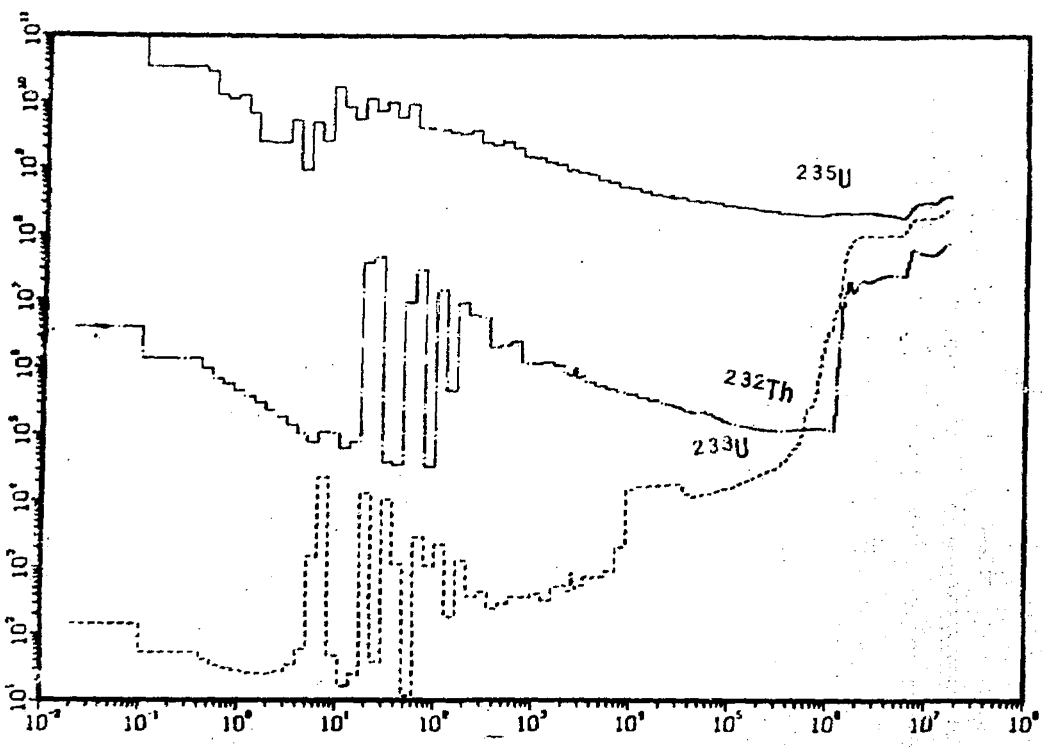

Fig. 3. Neutron kerma factors for ^{232}Th, ^{235}U, and ^{238}U

Table 4. Comparison of Neutron Kerma Factors in MACKLIB-IV[a] and MACKLIB[b] for Several Materials in Selected Energy Groups[c,d]

	13.499–14.918		10.0–11.052		1.0026–1.102	
Mat.	MACKLIB/IV	MACKLIB	MACKLIB/IV	MACKLIB	MACKLIB/IV	MACKLIB
Be	3.018	3.473	1.848	2.738	0.516	0.521
^{6}Li	4.901	4.400	4.760	4.154	1.684	1.782
^{7}Li	4.185	3.313	3.785	2.952	0.408	0.416
^{10}B	6.260	3.686	5.002	3.433	1.118	1.518
^{12}C	4.618	3.244	1.980	2.407	0.350	0.364
Al	6.252	4.010	2.852	2.893	0.148	0.206
Nb	1.207	1.045	0.764	0.792	0.082	0.093
Cu	3.517	2.712	1.898	1.994	0.096	0.101
Pb	0.282	0.266	0.232	0.252	0.041	0.047

[a]See Ref. 4.

[b]See Ref. 2.

[c]All MACKLIB kerma factors are based on ENDF/B-III data but those of MACKLIB-IV are based on ENDF/B-IV.

[d]All neutron kerma factors in units of MeV-barn/atom.

V. SUMMARY

Major developments have been maae in the calculational aogirthms and new capabilities have been added into the MACK computer program. The new version of the program, MACK-IV, is available for distribution. The program generates important nuclear response functions such as neutron kerma factors and tritium breeding and gas production functions as well as the gamma production cross sections. The new developments in MACK-IV represent a major step in ensuring energy conservation in nuclear heating calculations. The program is useful in almost all practical nuclear applications.

A new library, MACKLIB-IV, of nuclear response functions was generated using MACK-IV and basic nuclear data from ENDF/B-IV. The library includes data for a large number of materials of great interest in fusion, fusion-fission hybrids, and fission applications. The library and a retrieval routine are readily available from major nuclear information centers.

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