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by

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ABSTRACT

Formats have been proposed to allow the inclusion of evaluated neutron kerma factors in ENDF/B. The task of preparing evaluated kerma factors is analyzed in this report and is found to present numerous difficulties. Two alternative approaches to kerma-factor calculations are suggested, both of which require modifications of existing evaluations, notably through the inclusion of cross sections now missing for a number of neutron reactions, to allow postevaluation kerma-factor processing. The first approach requires neutron-induced charged-particle spectra, in addition to the missing reaction data. The second approach, which would not require the charged-particle spectra, would enforce energy conservation in the computed results.

I. INTRODUCTION

In a number of engineering applications, there has been increasing need for the calculation of factors which convert neutron fluence to kerma (kinetic energy release in materials). The kerma factor can be defined as the total neutron interaction cross section multiplied by the average value (per interaction) of the sum of the kinetic energies of the recoil nucleus and secondary charged particles. The kerma factor is a one-dimensional array, similar to a reaction cross section, and can be represented in fine detail on a continuous-energy basis or flux-averaged over neutron energy multigroups.

The availability of accurate kerma factors is important in such diverse areas as fusion reactor blanket design, biological dosimetry, fast neutron radiation therapy, and nuclear weapons effects. Most of these comments are directed toward the problem of the calculation of neutron heating in fusion reactor blankets, but the needs of the other applications mentioned are considered as well. In most of these areas, the neutron fluence is calculated using multigroup techniques, so that multigroup kerma

factors would appear to be adequate in the near term. Another common feature of these application areas is an interest in high-energy (14 MeV) neutrons as well as low-energy neutrons. In contrast to the lower energy region, where the kerma factor is dominated by one or two (usually well-known) reactions, at 14 MeV, elastic scattering, inelastic scattering, exothermic reactions, and endothermic reactions all contribute significantly to the kinetic energy release. This complexity has made the calculation of accurate kerma factors a problem of continuing interest.

A number of computer programs¹⁻³ have been written to calculate kerma factors. The most recent of these, MACK,¹ processes the neutron files from ENDF/B (or data in the same format) for all reactions which result in the release of significant amounts of charged-particle energy. Like most of its predecessors, MACK is a stand-alone program in that it can be operated independently of other nuclear data processing codes. This stand-alone feature, plus the previously mentioned complexity of kerma-factor calculations, has led to suggestions

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that MACK be used as part of the ENDF evaluation process to produce evaluated pointwise kerma factors. These pointwise kerma-factor data would be entered into ENDF/B as primary data. Multigroup kerma factors could then be processed by the usual multigroup processing codes, just as they process neutron reaction cross sections, during the process of producing neutron transfer matrices. This proposal has its merits, but as will be shown, it might cause more problems than it would solve.

II. KERMA-FACTOR COMPLICATIONS

To analyze the motivation behind the proposal to produce evaluated kerma factors, we describe below several sources of complexity in the calculation of kerma factors from ENDF/B basic data.

A. Missing Reaction Cross Sections

Many reaction cross sections, such as $\sigma_{n,p}$ and $\sigma_{n,\alpha}$, are missing for the heavier materials. This is important because, in the Fe-Mo region, (n,p) and (n, α) reactions are responsible for about 70% of the total neutron heating.¹

B. Incompletely Described Gamma-Ray Events

Gamma-ray production events are often incompletely described. For example, in the (n,n' γ) reaction, one must calculate the average energy released in the form of secondary neutrons and photons in order to calculate the kerma (proton plus recoil nucleus) by energy balance. If the photon corresponds to discrete level decay, the level can be indexed in the neutron file. Usually this level information is missing, and if the gamma-ray spectrum is a continuum, then there is not even a format for giving the spectrum in the neutron file. Alternatively, one could process the proton spectrum (which is formatted, but presently there is no proton spectral data in the files). A similar difficulty arises in (n,2n γ) events. Unless one knows the average energy of each neutron, one cannot calculate the recoil energy without approximation.

C. Computations from Beta Decay

The total energy deposition in a given material often includes a significant contribution from the beta decay of neutron-reaction products. In principle, one could calculate this decay heat using calculated neutron fluxes and a special-purpose decay heat code such as CINDER,⁴ but in CTR problems there has been a trend toward including the decay

heat in the kerma factor. The calculation of these "delayed-kerma" factors requires input data which are not included in the ENDF neutron and gamma-ray formats and files.

We now turn to a discussion of the problem areas listed above.

III. MISSING REACTION DATA

In the production of evaluated pointwise kerma factors, the problem of missing data could be handled by preparing a special-purpose library of model-generated reaction cross sections. When an important reaction is missing from a given ENDF evaluation, MACK could access this library to get the information needed to produce a sensible kerma factor.

The fact that some important cross sections have not been measured is not a strong argument for the production of evaluated kerma factors. It would seem preferable to add any new model-generated data for the (n,p) and (n, α) cross sections directly into the ENDF/B files as rapidly as possible, and then to run MACK (or a similar code) after the files have been updated. In this way, future revisions of these estimated cross sections would require that the evaluator revise just the cross sections in question and not the evaluated kerma factor as well. This approach would be a reasonable alternative to the inclusion of evaluated kerma directly in the ENDF/B files.

IV. GAMMA-RAY PRODUCTION PROBLEMS

The same sort of comment applies to the second difficulty mentioned above. If one uses model calculations to supply charged-particle energy spectra for the calculations of kerma factors, then those spectra should be inserted directly into the appropriate ENDF/B files (the MT = 700 series, in this case) where they can be easily inspected and revised whenever necessary. As in the case of the model-generated (n,p) and (n, α) cross sections discussed above, there are important applications, completely unrelated to kerma, which would benefit from the existence of evaluated neutron-induced charged-particle energy spectra in ENDF/B. For example, at the temperatures generally encountered in astrophysics, proton and alpha-particle ranges are comparable to neutron ranges, so that charged-particle transport is required.

It is possible that it will take several years to fill in the charged-particle spectrum files. In the meantime, it is important to note that kerma factors can be calculated without a full description of the charged-particle spectra. One can do this by using the gamma-ray production files where provided and using energy-balance relations. This approach, which offers a second alternative to putting kerma factors directly into the ENDF files, is developed in detail in the Appendix. It is vulnerable to two distinct objections; namely, (1) MACK is presently not coded to handle the gamma ray production files, and (2) gamma-ray production evaluations do not exist for many ENDF materials.

In response to the first objection, we note that there exist ENDF processing codes (e.g., LAPH-ANO⁵) which can process the ENDF/B gamma-ray data into a form suitable for the use of energy-balance techniques. Our response to the second point is that considerable momentum is developing to improve this situation. In ENDF/B-III only 11 evaluations contained gamma-ray production cross sections. In ENDF/B-IV, this will grow to about 35. Also, it should be noted that in neutron-transport problems not involving fission (e.g., fission-reactor shielding, fusion-reactor blankets, and a transport of weapons radiation) the gamma-ray heating is usually of the same order of magnitude as the direct neutron heating. Thus, there will be relatively few cases where neutron-heating (kerma) calculations will be made in the absence of gamma-ray production and transport calculations.

Just as in the MACK approach, the method outlined in the Appendix depends on the availability of cross sections for all important non-elastic reactions, such as (n,p), (n, α), (n,n'p), (n,2n), etc. In contrast to the MACK approach, the energy-balance method makes it possible for all reactions to be treated without approximation even if the angle and energy distributions of the charged-particle products are unavailable.

V. DELAYED KERMA FROM DECAY PROCESSES

For some nuclides and in some neutron energy regions, the kerma factor is dominated by particle emission (betas, alphas, conversion electrons, etc.) from neutron activation products. M. Abdou mentions¹ the striking example of ⁷Li. At low energies the

major energy-release mechanism is radiative capture, followed by rapid beta and alpha decays:

The charged-particle energy released in the beta and alpha decays is 9.31 MeV, while the capture gamma ray accounts for only 2.03 MeV. This strong dominance of decay heating over prompt (prior to beta-decay) heating is quite unusual in CTR neutronics calculations, but it does point up the fact that decay heating must be treated in some fashion, even if it is approximate. The information needed to assess decay heating is not contained in the present ENDF neutron and gamma formats and files. Further, the decay modes of activation products are widely varied. Thus, it appears that decay-heating data should be entered in the files by the evaluator.

Probably the most direct way to enter the decay-heating information is to flag the contributing neutron reactions and to enter the corresponding data in a separate file. For example, in the ⁷Li example given above, the capture cross section MT = 102 could be flagged to indicate the existence of significant decay-heating processes. At least three pieces of data would then be entered elsewhere in the neutron file. One would like to have (1) the characteristic decay time (0.8 seconds, in this example); (2) the average amount of delayed kerma per capture (9.31 MeV here); and (3) the average amount of delayed gamma-ray energy release per capture (~ 0 MeV here). If more than one activity is produced, resulting in a nonexponential decay-heat deposition rate, several of these three-number data sets could be entered for a given initiating reaction. The initial data for this short delayed-kerma file probably would be gathered in a rather ad hoc fashion. Eventually, however, one would expect an automated link between this file and the extensive ENDF/B decay-heating file now being formatted.⁶

VI. SUMMARY

We have examined three major reasons for adopting the proposal to include evaluated pointwise kerma factors in the ENDF neutron file. All three reasons can be reduced to the statement that the evaluated data in ENDF/B is inadequate for the calculation of accurate kerma factors. We feel that the

solution to this problem is to evaluate and add new differential data, wherever this is necessary to permit postevaluation kerma-factor processing. This will require revisions of many existing ENDF evaluations to include model-generated estimates of certain cross sections, as well as a format change to accommodate the delayed-kerma data.

In addition, if one chooses to produce kerma factors using only the neutron files using MACK (the first alternative), then one also needs evaluated charged-particle spectra for certain reactions. If one chooses to use both the neutron and gamma-ray files and energy-balance techniques (the second alternative), then the charged-particle spectra are not required for kerma calculations.

In either case considerable work will have to be done on the ENDF files to allow meaningful post-evaluation kerma calculations. It is felt, however, that this extra work is less than would be required under the original proposal to put evaluated kerma factors directly into the files. This conclusion is based on the following considerations: (1) the new microscopic data will be entered in the files explicitly making it easier to reevaluate and revise the data in the future; (2) the evaluator will not be burdened with the task of understanding and operating a complex kerma-factor processing code. In addition, the new microscopic data will be useful in other applications such as activation and transmutation. An advantage restricted to the energy-balance approach is that the calculated kerma fac-

tors will be consistent (from an energy conservation viewpoint) with the evaluated neutron and gamma-ray files.

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REFERENCES

1. M. A. Abdou, C. W. Maynard, and R. Q. Wright, "MACK: A Program to Calculate Neutron Energy Release Parameters (Fluence-to-Kerma Factors) and Multigroup Reaction Cross Sections from Nuclear Data in ENDF Format," Oak Ridge National Laboratory report ORNL-TM-3993 (1973).
2. J. J. Ritts, M. Solomito, and D. Steiner, "Kerma Factors and Secondary Gamma Sources for Some Elements of Interest in Thermonuclear Blanket Assemblies," Oak Ridge National Laboratory report ORNL-TM-2564 (1970).
3. R. L. Bach and R. S. Caswell, "Energy Transfer to Matter by Neutrons," *Radiation Research* **35**, 1, (1968).
4. T. R. England, "An Investigation of Fission Product Behavior and Decay Heating in Nuclear Reactors," *Trans. Am. Nucl. Soc.* **15**, 443 (1972).
5. D. J. Dudziak, R. E. Seamon, and D. V. Susco, "LAPHANO: A P_0 Multigroup Photon-Production Matrix and Source Code for ENDF," Los Alamos Scientific Laboratory report LA-4750-MS (ENDF-156) (1972).
6. R. E. Schenter, "Fission Product Subcommittee Report," an enclosure in "Summary of CSEWG Meeting of May 23-24, 1973," Brookhaven National Laboratory memorandum.

APPENDIX

THE ENERGY-BALANCE APPROACH

Neutron downscatter, gamma-ray production, and charged-particle energy release (kerma) are intimately related through the law of conservation of energy. The ENDF system is now committed to the goal of developing valid cross sections for the first two processes, so it is only natural to consider the use of energy-balance techniques to derive kerma factors from the existing neutron and gamma data.

In the following we denote by $\sigma_1(E)$ the cross section for a reaction of type 1 induced by a neu-

tron having energy E . The average value of the sum of the kinetic energies of the recoil nucleus and secondary charged particles we shall label C_1 . The average value of the sum of the energies of secondary neutrons will be labeled N_1 and the analogous quantity for gamma rays, G_1 .^{*} G_1 is assumed to include the contributions from long-lived gamma-emitting isomers. If an isomeric reaction product de-

^{*} σ_1 , C_1 , N_1 , and G_1 are all functions of the neutron energy E . Unless needed for clarity, we will henceforth drop the functional notation.

cays by beta emission, then production of that isomer is treated as a different reaction type i from the reaction to the ground state. Heat generation due to beta decay itself is considered separately (see Sec. V in the main text).

Under the ground rules set down above, Q_i , the "ground-state" Q -value of reaction type i satisfies the relation

$$Q_i = (N_i + G_i + C_i) - E \quad (1)$$

The kerma factor k_i for this reaction is defined as

$$k_i = \sigma_i \cdot C_i \quad (2)$$

and the total kerma factor K is obtained by summing over all possible reactions.

$$K = \sum_i k_i \quad (3)$$

Combining Eqs. (1)-(3) we have the basic energy-balance relation for kerma factor calculations,

$$K = \sigma_{\text{tot}} E + \langle \sum_i \sigma_i Q_i \rangle - \langle \sum_i \sigma_i N_i \rangle - \langle \sum_i \sigma_i G_i \rangle \quad (4)$$

where σ_{tot} is the usual total neutron cross section. All four of the terms on the right hand side of Eq. (4) can be computed fairly easily in a multigroup environment using the present ENDF neutron and gamma-ray processors at the same time as the multigroup transfer matrices are prepared. Should a standard ENDF continuous-energy gamma-ray production processor be developed in the future, only a modest extension of the continuous-energy neutron processors would be required to produce continuous-energy kerma factors using the energy-balance approach.

To clarify what we mean by ground state Q -value, Q_i , we consider some concrete examples. Q_i for both elastic and purely $(n,n'\gamma)$ inelastic scattering is zero. Further, the Q_i 's for (n,p_0) , (n,p_1) , $\dots(n,p_k) \dots$, where the subscript indicates the excited state of the recoil nucleus, are all the same.* Thus, to evaluate the Q -value term in Eq. (4) what is needed is the "total" cross section for all important nonscattering reactions. By "total" here we mean the sum over all states of excitation of the residual nucleus. For example,

$$(\sigma_{n,p})_{\text{total}} = \sigma_{n,p_0} + \sigma_{n,p_1} + \dots + \sigma_{n,p_k} + \dots$$

* The reaction (n,p_k) here does not include the reaction in which level k decays by neutron emission, for example. That process is assumed to be included in the $(n,n'p)$ cross section.

These cross sections are the usual reaction cross sections included in the ENDF/B files. Some of the more important reactions are listed in Table I along with the assigned ENDF/B MT number.

TABLE I

SOME IMPORTANT NONSCATTERING REACTIONS IN ENDF/B

MT	Reaction	MT	Reaction
16	(n,2n)	102	(n, γ)
22	(n,n' α)	103	(n,p)
24	(n,2n α)	104	(n,d)
28	(n,n'p)	107	(n, α)

It has been noted earlier that these reaction cross sections are often missing in ENDF/B especially for the heavier nuclides. We feel that this situation should be remedied as rapidly as possible through the use of nuclear model calculations where necessary. These cross sections are important not only for kerma-factor calculations, but also for transmutation and activation calculations. In fact, these total reaction cross sections are just what one normally measures in an activation cross section measurement.

A complication arises from the fact that the nuclear Q -value of a given reaction is isotope-dependent. If the reaction cross section is summed over isotopes, then the value of Q_i which one should use in Eq. (4) depends on the fraction of the reactions due to each isotope, that is, Q_i becomes a function of E . As long as the reaction cross sections are separated by isotope, however, Q_i is a single number, which is already formatted for the ENDF/B reactions given in Table I. (In order to make the energy-balance approach meaningful, however, these Q -values need to be carefully reviewed for accuracy and consistency.) For obvious reasons, transmutation and activation calculations also require the reaction data for individual isotopes. Thus it appears desirable to present the reaction data on an isotope-by-isotope basis in future evaluations. For the present purposes, it does not appear necessary to present the neutron downscatter and gamma-ray production cross sections for individual isotopes. If the neutron and gamma-ray data apply to a mixture of isotopes, then the σ_i in Eq. (4) should be multiplied by the appropriate atom frac-

tion and the sum on i extended over the number of isotopes present as well as over reaction types.

As a general comment, it should be noted that the use of this energy-balance technique places new demands on the overall consistency of the evaluated neutron and gamma-ray data. For example, if the energy spectrum of the secondary neutrons or gammas is too hard, then from Eq. (4) we see that the calculated kerma factor could very well become negative. We do not feel that this situation is neces-

sarily undesirable. For one thing, this kind of calculation will rapidly point out areas where the neutron and gamma-ray files are unrealistic. Prior to the revision of the unrealistic neutron and/or gamma-ray data, the use of a kerma factor which enforces energy conservation would appear to be preferable to using one which is more reasonable standing alone, but which is inconsistent with the neutron and gamma-ray data.