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AUTHOR(S): R. C. Little and R. E. Seamon

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Los Alamos National Laboratory
Los Alamos, New Mexico 87545

NEUTRON-INDUCED PHOTON PRODUCTION IN MCNP

R. C. Little and R. E. Seamon
Los Alamos National Laboratory
University of California
Los Alamos, New Mexico, United States

ABSTRACT

An improved method of neutron-induced photon production has been incorporated into the Monte Carlo transport code MCNP. The new method makes use of all partial photon-production reaction data provided by ENDF/B evaluators including photon-production cross sections as well as energy and angular distributions of secondary photons. This faithful utilization of sophisticated ENDF/B evaluations allows more precise MCNP calculations for several classes of coupled neutron-photon problems.

I. INTRODUCTION

Coupled neutron-photon transport problems often require the use of Monte Carlo calculations. An important aspect of such calculations is the production of photons at neutron collisions. The neutron-induced photon production should be a faithful representation of the nuclear data evaluation. In particular, it is necessary to sample adequately the given energy and angular distributions of the secondary photons. A method is described here for improved neutron-induced photon production in the Monte Carlo code MCNP. The method is completely continuous in both incident neutron energy and outgoing photon energy, and faithfully preserves the intentions of evaluators.

II. MCNP

MCNP[1] is a general-purpose, continuous-energy, coupled neutron-photon Monte Carlo transport code maintained by the Radiation Transport Group at the Los Alamos National Laboratory. The code may be run in any of three modes: neutron transport only, photon transport only, or combined neutron-photon transport. It is this last mode that we concern ourselves with in this paper.

In a coupled neutron-photon problem in MCNP, a specified neutron source is transported through the geometry of the problem. Photons are produced at neutron collisions, and are subsequently transported through the geometry as well. Since it is these neutron-induced photons that serve as the effective photon source in the problem, the accuracy of the ensuing photon transport and of any photon tallies can be no better than the accuracy of the initial description of the photons. The accuracy of the production of photons is measured by how well the characteristics of the secondary photons produced match the specifications of the nuclear data evaluation being used.

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MCNP has access to nuclear data from libraries in ACE (A Compact ENDF) format. ACE libraries are produced in Group T-2 at Los Alamos from ENDF/B-format evaluations using the nuclear data processing code NJOY.[2] For production versions of MCNP up to and including Version 2C (before February, 1983), a limited amount of photon-production data was available in the ACE libraries. For each isotope, the total photon-production cross section was tabulated as a function of neutron energy. These total photon-production cross sections allowed the proper number (or weight) of photons to be produced at neutron collisions. However, the only information on the ACE libraries concerning the secondary photons for a particular isotope was a 30x20 matrix of photon energies; for each of 30 incident neutron energy groups, 20 equally probable photon energies were specified. All photons were produced isotropically in the laboratory system. This limited data available in ACE format meant that a wealth of photon-production information contained in ENDF/B-format evaluations was not available to MCNP.

We will next describe briefly the photon-production information contained in ENDF/B-format evaluations.

III. PHOTON-PRODUCTION DATA IN ENDF/B EVALUATIONS

It is obvious that the total neutron cross section is the sum of several partial neutron cross sections. In ENDF/B,[3] data are provided in Files 2-5 (MF=2,3,4,5) for the cross sections for each neutron reaction, as well as the energy and angular distributions of any secondary neutrons produced in each reaction. All of these data for each of the partial neutron reactions are incorporated into ACE libraries and are used by MCNP.

Similarly, the total photon-production cross section is the sum of several partial photon-production cross sections. In ENDF/B, data are provided in Files 12-15 (MF=12,13,14,15) for the cross sections for each photon-production reaction, as well as the energy and angular distributions of the secondary photons produced in each reaction. In the past, these data were not all incorporated into ACE libraries (see Section II), and therefore were not all used by MCNP.

Each partial photon-production reaction is attributed to a particular neutron reaction, for example, (n,2n), (n,fission), (n,p), etc. The cross section for a particular partial photon-production reaction may be either (1) the cross section for the production of a discrete-energy photon, or (2) the cross section for the production of a spectrum of photons. One neutron reaction may lead to the production of several discrete-energy photons; hence, that one neutron reaction would be responsible for several partial photon-production cross sections.

The magnitude of information available is indicated by using the example of the ENDF/B-V evaluation of ^{27}Al (MAT=1313, Tape=506). The evaluation includes cross sections for 30 partial photon-production reactions from neutron inelastic scattering (29 discrete photons and 1 continuum spectrum of photon energies), 9 partial photon-production reactions for (n,n')p (8 discrete, 1 continuum), 4 partial photon-production reactions for (n,p) (all discrete), and 89 partial photon-production reactions for radiative capture (all discrete). Thus, a total of 132 partial photon-production reactions exist for

^{27}Al, each of which has associated with it a cross section, energy distribution, and angular distribution. Furthermore, each of these last three quantities may be a function of neutron energy. From this example, one may understand the logic behind the original simplifying model in MCNP of a 30x20 matrix of photon energies to be sampled for the production of neutron-induced photons. Unfortunately, the model is a limiting factor in the accuracy of certain MCNP calculations. With the arrival of faster machines and increased memory, it is possible to include and sample from all of the detailed photon-production information available.

IV. EXPANDED ACE LIBRARIES FOR MCNP

Starting with Version 2D (February, 1983), MCNP has access to cross-section libraries that include detailed photon-production information. We call such libraries "expanded ACE libraries" and proceed here to describe their contents and relationship to MCNP.

A processing code called ADDGAM has been written that merges the former ACE libraries with information from the appropriate ENDF/B tapes to produce expanded ACE libraries. The expanded libraries contain completely new sections with partial photon-production reaction information. ADDGAM processes the following data from ENDF/B files: photon multiplicities (MF=12,LO=1), photon transition probability arrays (MF=12,LO=2), photon-production cross sections (MF=13), photon angular distributions (MF=14), discrete photon energies (MF=12,13), and continuum photon energy spectra (MF=15). The strategy used when deciding on a format for the expanded section of the libraries was to incorporate the photon-production reaction information in as nearly the same form as possible as the original neutron reaction information. For 55 materials from ENDF/B-V, the total length of the expanded ACE library is 12.5% greater than the length of the same materials on the previous ACE library.

A. Photon-Production Cross Sections

The format of ENDF/B allows photon-production cross sections to be specified in two ways: (1) the energy-dependent production cross sections may be given directly, or (2) energy-dependent multiplicities may be given, with the understanding that the production cross section as a function of neutron energy is equal to the product of the energy-dependent multiplicity and a specific energy-dependent neutron reaction cross section. The data from ENDF/B are carried over to expanded ACE format in whichever form they are originally specified. If production cross sections are given directly in ENDF/B, they are simply transferred onto the previously existing ACE energy grid. When multiplicities are given, the (neutron energy, multiplicity) pairs as well as the specified interpolation scheme are written to the expanded ACE library. The neutron reaction cross sections, by which the multiplicities must be multiplied to determine production cross sections, are already contained in the previous ACE format.

When producing a photon, the partial photon-production reaction responsible for the photon, "I", is determined in MCNP from:

$$\sum_{J=1}^{I} \sigma_{\gamma,J}(E) > \xi\, \sigma_{\gamma,tot}(E) \geq \sum_{J=1}^{I-1} \sigma_{\gamma,J}(E)$$

where E is the incident neutron energy, $\sigma_{\gamma,J}$ is the photon-production cross section for partial reaction J, ξ is a random number on (0,1), and $\sigma_{\gamma,tot}$ is the total photon-production cross section. Once reaction "I" is chosen, distributions appropriate to reaction "I" are sampled to determine the direction and energy of the secondary photon.

B. Photon Energy Distributions

The previous 30x20 matrix of neutron-induced photon energies (see Section II) is inadequate for three reasons: (1) discrete photon lines are not faithfully reproduced, (2) the high-energy (low-probability) tail of a continuum photon energy distribution is not well sampled, and (3) the multigroup representation is not consistent with the continuous-energy nature of MCNP.

Figure 1 illustrates some problems associated with the previous 30x20 matrix of photon energies. The plot is for titanium (ENDF/B-V) with an incident neutron energy of 1.0E-11 MeV. The histogram is the secondary energy

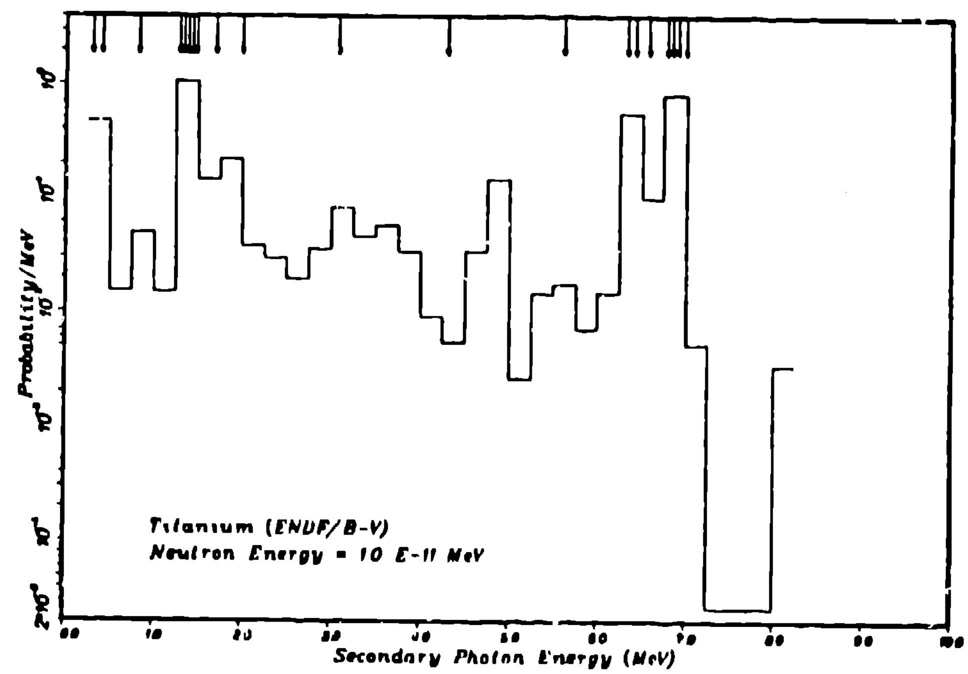

Fig. 1. The secondary photon energy distribution for radiative capture on titanium. The histogram is the spectrum given in ENDF/B-V for an incident neutron energy of 1.0E-11 MeV. Each of the arrows at the top of the curve indicates one of the 20 equally probable photon energies used to represent the histogram distribution in the original ACE format.

spectrum specified in the evaluation (for radiative capture, the only reaction producing photons at this energy). The 20 arrows at the top of the plot represent the 20 equally probable photon energies contained on the ACE library for the lowest-energy neutron group. The difficulty in representing a continuous spectrum with discrete energies is evident. Not evident in the simple example shown in Fig. 1 are the additional difficulties of using 20 discrete energies to represent a combination of many photon energy distributions integrated over a neutron energy group.

The biggest advantage of expanded ACE format is that MCNP now has enough information available to sample the secondary photon energies exactly as the evaluator intended. After the code has used the partial photon-production cross sections to sample the partial photon-production reaction, the secondary photon energy distribution corresponding to that reaction is sampled. Recall that there are only two types of photon energy distributions allowed in the format of ENDF/B: discrete energies and tabulated spectra.

The discrete energy photons are, of course, trivial to sample. The secondary photon energy, E_g', is simply calculated as either

$E_g' = E_g$ (non-primary photon)

or $E_g' = E_g + \{A/(A + 1)\} * (E_n)$ (primary photon)

where A is the atomic weight ratio of the target material and E_n is the incident neutron energy. The parameter, E_g, given by the evaluator, is the secondary photon energy for non-primary photons or the binding energy for primary photons. Discrete photons are often valuable in the sense that they are signatures of a particular isotope. These signature photons now may be easily used to compare experimental results to MCNP calculations.

The second type of distribution is a tabulated spectrum of secondary photon energies, for example the histogram in Fig. 1. The interpolation between adjacent photon energy points is specified to be either histogram or linear-linear. Tabulated distributions are sampled exactly in MCNP for both interpolation schemes.

C. Photon Angular Distributions

Most secondary photons from ENDF/B-V evaluations are specified to be produced isotropically in the laboratory system, as was assumed in the old version of MCNP. There are exceptions, however, including secondary photons from certain reactions with C, ^{14}N, and ^{16}O.

The current version of MCNP no longer assumes that all neutron-induced photons are produced isotropically. All non-isotropic photons have their angular distributions represented in expanded ACE format by 32 equally probable cosine bins. This is the same treatment given to secondary neutron angular distributions. An example of a secondary photon angular distribution for Carbon is shown in Fig. 2. The photon is from the (n,n') reaction with an incident neutron energy of 7.5 MeV. The solid curve is the distribution as given in ENDF/B-V; the histogram represents the 32 equally probable cosine bins sampled by MCNP.

D. Summary of Expanded ACE Libraries in MCNP

The advantages to MCNP of having access to photon-production data in expanded ACE format are suggested by Fig. 3. With ACE format alone (left side

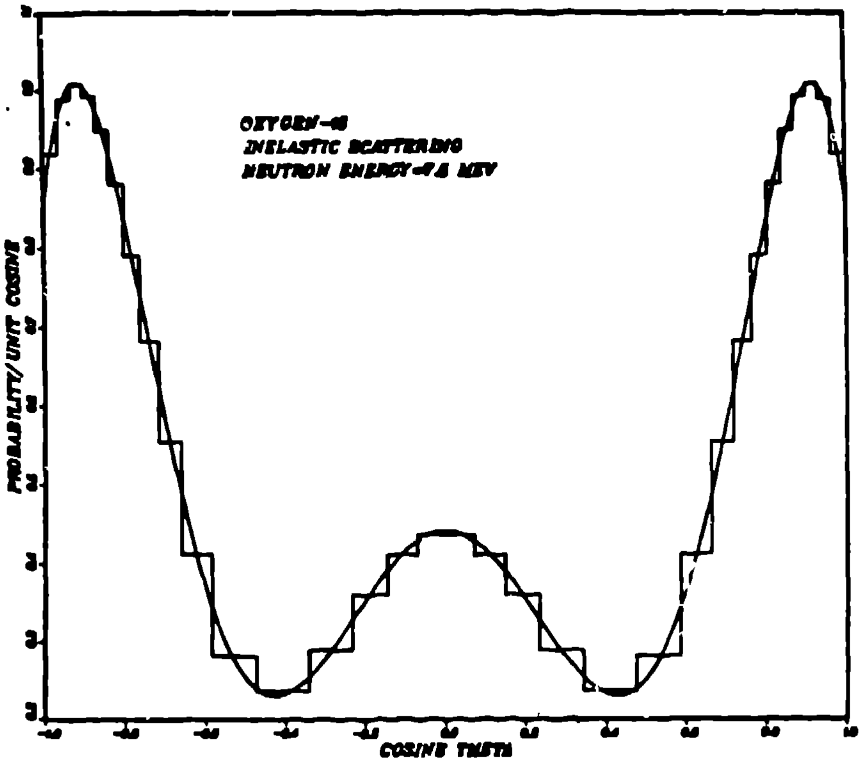

Fig. 2. The angular distribution for secondary photons from inelastic scattering on ^{16}O. The smooth curve is the given distribution in ENDF/B-V for an incident neutron energy of 7.5 MeV. The histogram is the 32 equally probable cosine bin representation used in expanded ACE format.

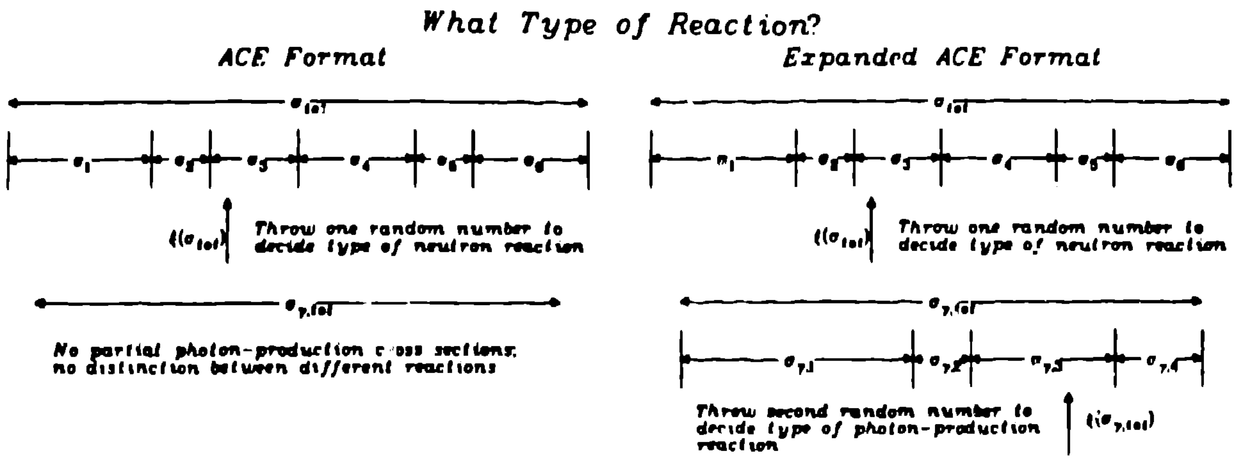

Fig. 3. The procedures for selecting the type of neutron reaction and type of photon-production reaction at a neutron collision. The left-hand-side is MCNP Version 2C with the original ACE format; the right-hand-side is MCNP Version 2D with expanded ACE format.

of Fig. 3), there is a sharp contrast between the mechanisms used to sample neutron reactions that produce secondary neutrons, and those that produce secondary photons. The neutron reactions are sampled exactly, and any secondary neutrons produced leave the collision with energies and directions sampled from distributions appropriate to the particular reaction. Conversely, there are no photon-production reactions to sample; hence no secondary photon distributions specific to particular reactions.

With expanded ACE format (right side of Fig. 3), there is complete symmetry between the mechanisms used to sample neutron reactions and photon-production reactions. The photon-production reactions are sampled exactly, and any secondary photons produced leave the collision with energies and directions sampled from distributions appropriate to the particular reaction. As Table 1 indicates, the precision of secondary photon production in MCNP is now commensurate with that of secondary neutron production.

Notice that two random numbers are used, one to choose the neutron reaction, and one to choose the photon-production reaction. The types of collisions are completely uncorrelated. For example, one might sample an (n,2n) reaction with ^{235}U, and then decide that a photon produced at the same collision was the result of a fission reaction. This method is perfectly acceptable as long as one is not trying to conserve integral quantities on a per-collision basis. In fact, this method is generally the only method available. It is required because of the way data are presented in ENDF/B evaluations, which itself is based on the way experiments are carried out. Particularly at high neutron energies, it is difficult to distinguish a photon produced from an inelastic scattering reaction with one produced from an (n,2n) reaction or with one produced from radiative capture, etc. Thus experimentalists tend to report, and evaluators tend to present, one neutron energy dependent photon-production cross section and one secondary photon energy spectrum from "all" neutron reactions, rather than several production cross sections

Table 1. MCNP Sampling of Physical Properties of Neutron Collisions

	Neutron Reaction	Photon-Production Reaction (ACE Format)	Photon-Production Reaction (Expanded ACE Format)
Type of Reaction	EXACT	NOT SAMPLED	EXACT
Number of Secondary Particles	EXACT	EXACT	EXACT
Secondary Angular Distributions	VERY GOOD	NOT VERY GOOD	VERY GOOD
Secondary Energy Distributions	VERY GOOD	NOT VERY GOOD	EXACT

and spectra from specific neutron reactions. So it is very difficult, if not impossible, to completely correlate the neutron reaction with the photon-production reaction.

There is a time penalty associated with the use of expanded photon-production data in MCNP. This penalty is extremely problem dependent, varying with such factors as what materials are in a problem and what energy spectrum of neutrons is involved. Typically, however, one may expect a 10–15% increase in running time.

V. RESULTS

Many problems have been run using the new method of photon production in MCNP. In Fig. 4, we illustrate the improvement observed in calculation of the neutron-induced photon leakage from a 20-cm radius magnetite (^{16}O,Ti,Fe) sphere with a central 14-MeV neutron source.[4] The photon leakage is plotted as a function of photon energy group. Group 1 is from 9-20 MeV and Group 12 is from 0.01–0.1 MeV. The solid line represents results from the ONETRAN discrete ordinates code[5] while the dashed line is from MCNP. The upper plot highlights obvious problems with the old MCNP photon-production method. There is a complete lack of agreement between MCNP and ONETRAN for photon energies greater than 2 MeV. The MCNP curve in the lower plot has been calculated with expanded photon-production data; the agreement between MCNP and ONETRAN is quite good.

Several types of calculations benefit from faithful reproduction of discrete-energy photon lines, in particular any calculation in which a discrete line is used as a signature of an isotope. With expanded photon-production data, the effective resolution of MCNP is perfect for discrete lines. The improvement is apparent in Fig. 5 where we plot the neutron-induced photon leakage spectrum from a 11.2-cm radius Cu sphere with a central 14-MeV neutron source. The solid line is MCNP with expanded photon production; the dashed line is MCNP without expanded photon production. At first glance, there appear to be many more discrete lines represented with the old calculational method, but most of these are simply manifestations of the 30x20 matrix of photon energies. Conversely, the peaks in the spectrum calculated with expanded photon-production data are real, representing discrete photon energies from Cu of 0.67, 0.77, 0.962, 1.115, and 1.326 MeV. (The 0.511 MeV annihilation peak is evident in both curves.)

VI. CONCLUSIONS

The amount of photon-production data available to MCNP prior to expanded ACE format cross-section libraries was clearly inadequate for certain classes of coupled neutron-photon transport calculations. The inclusion of detailed photon production information in expanded ACE libraries, and the use of this information in MCNP, has greatly improved the situation.

All difficulties associated with the previous 30x20 matrix of neutron-induced photon energies (see Section IV.B) have been eliminated, in particular: (1) discrete photon lines are faithfully reproduced, (2) continuum

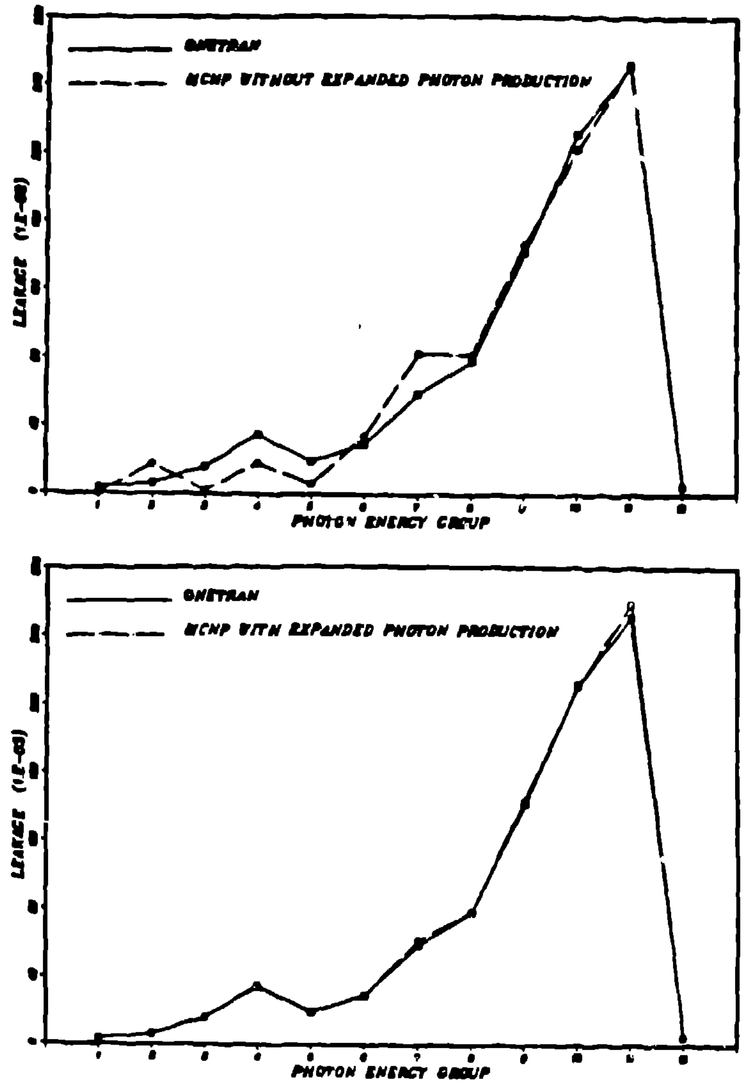

Fig. 4. Calculated photon leakage spectra from a magnetite sphere with a central 14-MeV neutron source. Group 1 is from 9-20 MeV and Group 12 is from 0.01-0.1 MeV. In both curves, the solid line represents results from the ONETRAN discrete ordinates code while the dashed line is from MCNP. The MCNP results in the upper curve were calculated with data in the original ACE format; those in the lower curve were calculated with data in expanded ACE format.

photon energy distributions are sampled exactly, and (3) the production of photons is completely continuous in both incident neutron energy and secondary photon energy.

The glory of Monte Carlo transport codes is that one may model the geometry and particle transport in difficult problems nearly exactly. In reproducing the intentions of evaluators, the nuclear data should be used in a manner that is no less exact. The method described here of handling photon

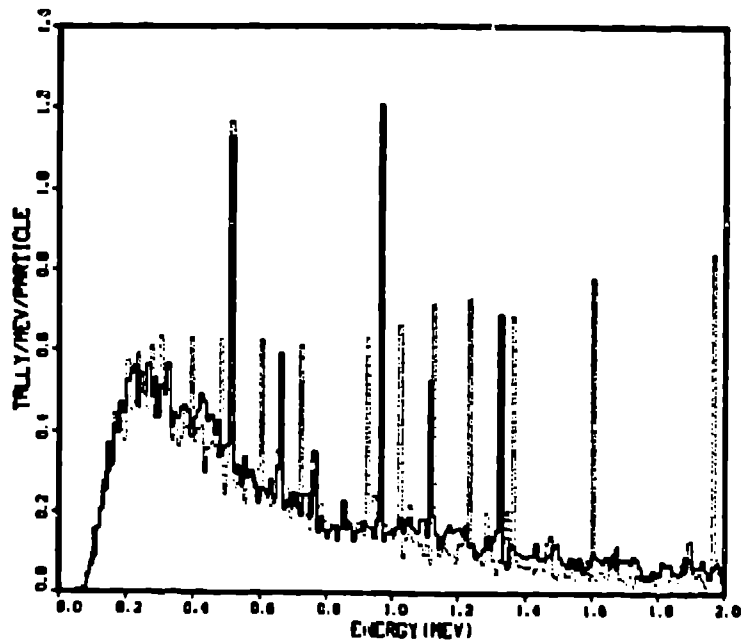

Fig. 5. Neutron-induced photon leakage spectrum from a Cu spher . The solid line is MCNP with expanded photon-production data; the dashed line is MCNP with data in the original ACE format.

production at neutron collisions is a significant advancement in the faithful utilization of sophisticated ENDF/B evaluations.

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