LA-UR-79-2848

MASTER

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SUBMITTED TO: International Conference on Nuclear Cross Sections for Technology, Knoxville, Tennessee
October 22-26, 1979

University of California

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Form No. 836 R3
St. No. 2629
12/78

UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36

VERIFICATION OF PHOTON-PRODUCTION PROCESSING TECHNIQUES

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Several laboratories have independently developed computer codes which use evaluated data from the ENDF/B file to produce group-averaged cross sections and transfer matrices for neutron-induced photon production. There have been several instances in which these codes have produced discrepant data sets, thereby casting doubt on the validity of all the codes. For a series of specified test cases, the results from three of these codes (NJOY, LAPHNGAS, and MACK-IV) were systematically compared with each other and with hand calculations. Several shortcomings in the codes have been discovered and repaired. One major difference of philosophy has been resolved. Consequently, the codes have arrived at substantial agreement on all of the nearly 1200 nonzero group constants calculated in the study.

(Photon-production, multigroup, code comparison, ENDF/B-IV)

Introduction

For several years, the LAPH series of codes were the most widely used photon-production processors of ENDF/B data. Versions of LAPH are in use at the Los Alamos Scientific Laboratory (LASL) [LAPH, LAPHANO] and General Atomic (GA) [LAPHANO]. Discrepancies in the LASL version of LAPHANO were reported by Seamon[1] at the September 1975 meeting of the Shielding Subcommittee (SSC) of the Cross Section Evaluation Working Group (CSEWG). Seamon's report included sample data from LAPHANO and comparisons with hand calculations. Several specific code modifications were also suggested to rectify the discrepancies.

Extensive modifications were made to the LAPHANO code at the Oak Ridge National Laboratory (ORNL) to give the LAPHNGAS code. LAPHNGAS was incorporated into the AMPX system—a modular system for producing coupled multigroup neutron-gamma cross section sets from ENDF/B data.*

In recent years, a number of other codes (NJOY,** MACK-IV) have gained the capability of processing photon-production data into transfer matrices in several Legendre orders. Because these codes were not related to LAPH, the opportunity was now available for intercomparison of independent codes and methods, as well as comparison of each code with selected hand calculations.

Under the auspices of the Shielding Subcommittee, the authors have compared calculated photon-production data from NJOY, MACK-IV, the LASL version of LAPHANO, the ORNL LAPHNGAS, and a late 1977 version of LAPHNGAS from the EG&G-Idaho version of the AMPX system. For the purpose of this paper, only NJOY, MACK-IV, and the ORNL LAPHNGAS will be discussed. The corrections made to LAPHNGAS as a result of this study are applicable in general to all LAPH-series codes. In the following discussions, it is assumed that the reader is familiar with the ENDF terminology described in Ref. 2.

Methodology

The scope of the study, summarized in Table I, was similar to the work of Seamon, except for the fact that higher order matrices were calculated for ..., ..., and ^{16}O. Isotopes and reactions were chosen to represent a variety of ENDF interpolation schemes. Photon-production data for both discrete and continuum photons were calculated using both multiplicities (MF12) and photon-production cross sections (MF13). In addition, a reasonably complex cascade of transition probability arrays was processed for ^{23}Na. To illustrate the complexity of the ^{23}Na transition probability data, the MT60 cascade is depicted in Fig. 1. The LASL 30-neutron and 12-photon energy group structures were used in this study. All calculations were repeated with both a constant and a 1/E neutron flux weighting for all Legendre orders. These simple weight functions were chosen to facilitate hand calculations. A total of 1168 nonzero matrix elements were compared.

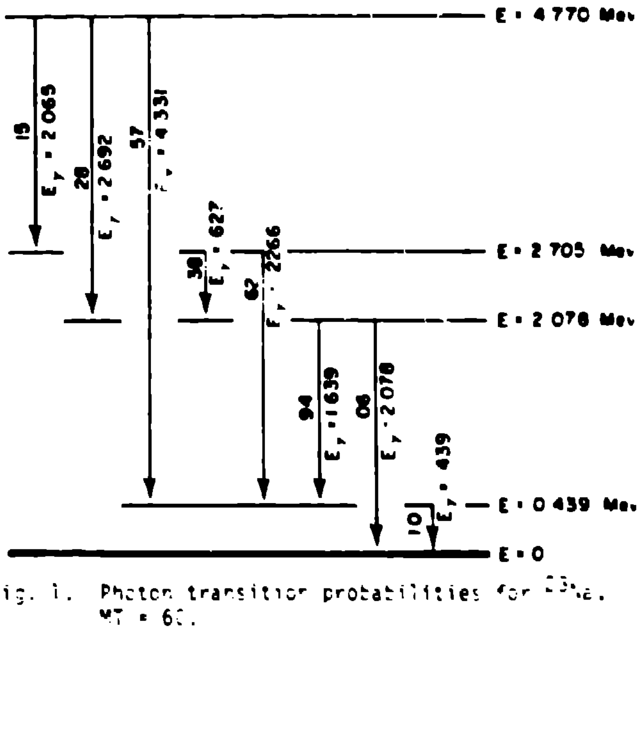

Fig. 1. Photon transition probabilities for ^{23}Na, MT = 60.

*The AMPX system is distributed by the Radiation Shielding Information Center (RSIC) in the package identified as PSR-63/AMPX-II.

**NJOY is a comprehensive computer code package for producing pointwise and multigroup neutron and photon cross sections from ENDF/B evaluated nuclear data.

TABLE I

ISOTOPES AND REACTIONS CONSIDERED IN THIS STUDY

Isotope	ENDF/B-IV MAT	MT	Photon Production Data: MF=12/13	LF[a]	E_{INT}[b]	MF = 15: E_{INT}[b]	$E_{i,INT}$[b]	Legendre Order
C-12	1274	51	13	DISC	2	-	-	P4
N-14	1275	102	12	DISC	2	-	-	P2
O-16	1276	4	13	DISC	2	-	-	P6
		22	13	DISC	2	-	-	P0
F	1277	3	13	CONT	1	2,4	1	P0
		4	13	DISC	2,4	-	-	P0
		102	13	CONT	5	1	1,2	P0
		107	13	DISC	2,4	-	-	P0
NA-23	1156	55	12	TPA	-	-	-	P0
		60	12	TPA	-	-	-	P0

[a]Photon distributions are discrete (DISC) or continuous (CONT) or the neutron energy dependence is represented by means of transition probability arrays (TPA).

[b]Interpolation scheme used in the evaluated data; that is, INT = 1, 2, 4, and 5 specifies constant, linear-linear, log-linear, and log-log interpolation schemes, respectively.

The calculations were performed on ENDF/B-IV evaluated data, which had been linearized, resonance-reconstructed and Doppler-broadened to 300 K using the NJOY code at LASL. The purpose of this preprocessing was to minimize the possibility of discrepancies arising from code differences not directly related to photon-production processing. Calculated matrices from all the laboratories were automatically sorted and compared at LASL. Side-by-side listings of all the calculated data were provided to all participants. In addition, the percentage difference by which each code deviated from the NJOY result was calculated and displayed. Discrepancies of less than 0.1 were set equal to zero. Cases in which the magnitude of the difference between two calculated cross sections was less than 1.0×10^{-6}b were similarly disregarded. The choice of NJOY as the standard of comparison was completely arbitrary.

Conclusions

The first round of comparisons showed agreement (to within 1) among the three codes for only 77 of the 1168 numbers calculated, a fact which reinforced our motivation for doing the study. Hand calculations performed on a representative sample of discrepant matrix elements suggested several improvements, and progress in the form of code modifications came quickly. The remaining discrepancies (involving 4 of the calculated numbers) are due in part to differences in interpretations of the ENDF/B-IV format or to minor differences in the calculational techniques used by the codes.* Three of these differences bear mentioning.

The most serious ambiguity exists in the processing of continuous energy spectra which are expressed in ENDF/B as normalized probability distributions $g(E_\gamma \leftarrow E_i)$ at selected neutron energies E_i. The codes under study employ different methods for interpolating to determine the photon spectra at intermediate neutron energies. The problem is illustrated in Figs. 2(a) and (b). At the lower neutron energy E_i, the photon endpoint energy is E_γ^i; at the higher neutron energy E_{i+1}, the photon endpoint energy is E_γ^{i+1}. At the intermediate neutron energy E_i', the NJOY and LAPHNGAS codes interpolate in such a way [Fig. 2(a)] as to give photon yields (dashed line) for photon energies up to E_γ^{i+1}, whereas the interpolation method used by MACK-IV [Fig. 2(b)] gives photon yields only up to an energy of E_γ^i. Because the resulting intermediate distributions are normalized, the NJOY/LAPHNGAS method gives more

*In addition, there are differences due to evaluation errors.

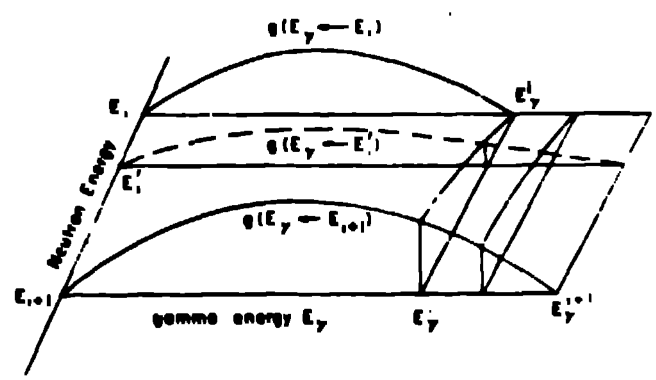

Fig. 2(a). NJOY/LAPHNGAS approach for interpolation of normalized probability distributions.

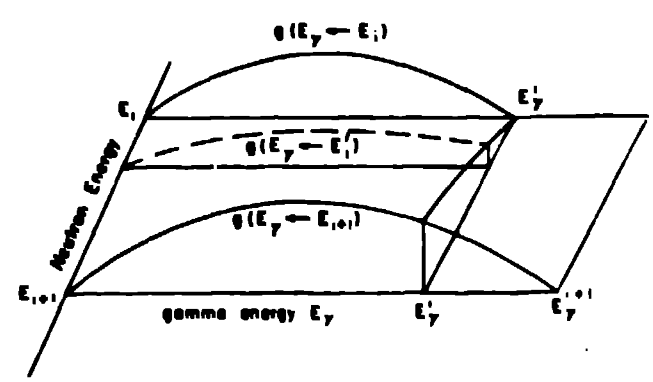

Fig. 2(b). MACK-IV approach for interpolation of normalized probability distributions.

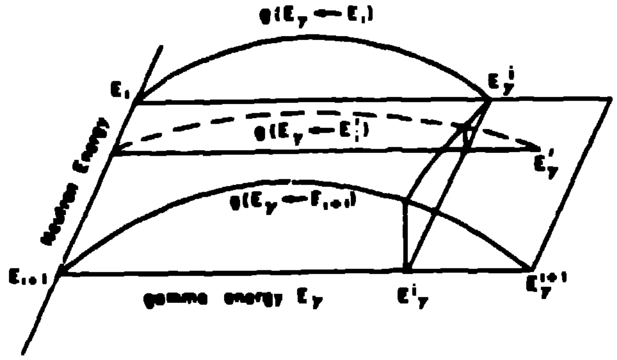

Fig. 3. Illustration of the proposed approach to interpolation of normalized probability distributions where $E_\gamma^{\prime}$ is defined from given TAB1 data.

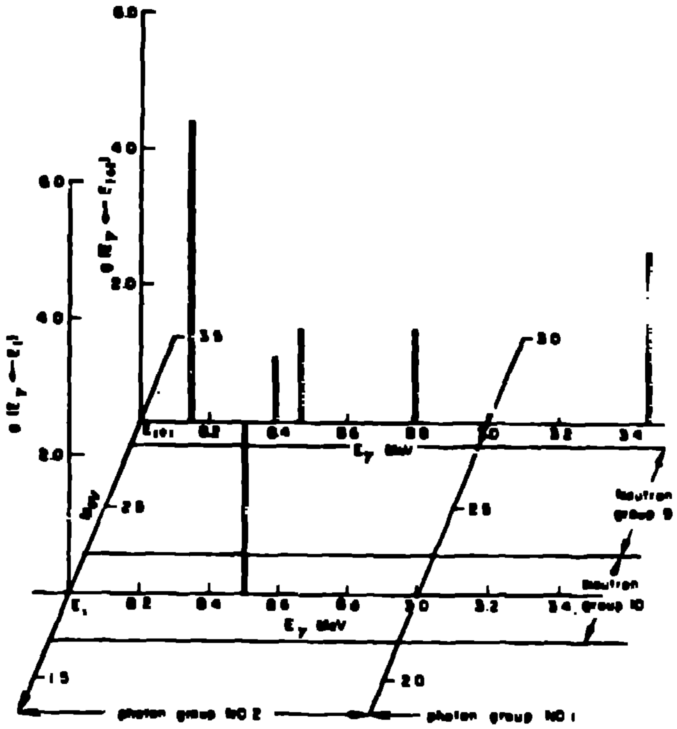

Fig. 4. Representative normalized probability distribution functions $g(E_\gamma \leftarrow E_i)$ for fluorine (MAT1277, MT102).

photons in higher energy groups and the MACK-IV method gives fewer photons in the same energy groups.

Neither the NJOY/LAPHNGAS nor the MACK-IV method gives a physically correct result. The endpoint energy for the intermediate photon spectrum should be somewhere between E_γ^i and E_γ^{i+1}. However, the current formats and procedures for ENDF/B-IV do not allow for an interpolation scheme that would produce the physically reasonable result.

A quick remedy for this ambiguity is to introduce a TAB1 record that gives the photon endpoint energy as a function of neutron energy. As shown in Fig. 3, the new data, which are compatible with current ENDF formats and which employ standard ENDF interpolation schemes, would allow a more reasonable method of interpolation.

A further source of difficulty with the normalized probability distributions is the use of this format to represent discrete photons. Figure 4 depicts the spectrum for MT = 102 in fluorine. Differences in the approach to interpolation, described above, led to a discrepancy (MACK-IV results versus NJOY/LAPHNGAS results) of 13 in photon production from neutron group 9 to photon group 2 and 100 from neutron group 9 to photon group 1. Similar difficulties were encountered in several neutron groups for this reaction. The effects of these discrepancies on the photon energy per neutron group were caluclated at ANL and found to be as high as 14 . These discrepancies, which can be significant for many applications, demonstrate the difficulties that can result from the use of file 15 to represent discrete photons.

A second difference involves the way in which the energies of certain discrete photons are calculated. The ENDF/B format calls for the photon energy E_γ to be calculated from the target atomic mass ratio AWR and the neutron energy E_n according to the formula

$$E_\gamma = E_\gamma' + \frac{AWR}{AWR+1} \times E_n ,$$

where E_γ' is the discrete photon energy listed in the ENDF file. The MACK-IV and NJOY codes calculate E_γ at each neutron energy within a group, whereas LAPHNGAS calculates one value of E_γ using the group-average neutron energy $\bar{E}_n$. The latter procedure can distort the average photon secondary energy by placing discrete photons in the wrong energy group. This difference is known to have caused a discrepancy in two of the 1168 nonzero group constants produced in this study--photon production from neutron group 5 to photon group 1 for radiative capture (MT = 102) in nitrogen for both constant and 1/E weighting.

Finally, there is a difference in the method of interpolating a function that is a product of two or more variables for which interpolation schemes are specified in ENDF. The MACK-IV code uses the highest interpolation scheme, while NJOY and LAPHNGAS use linear interpolation and disregard the interpolation schemes associated with the components of the product. When 1/E weighting is used, this difference in algorithm causes a maximum discrepancy of 0.5 for photon production from radiative capture (MT = 102) in nitrogen.

With the exceptions noted above, the three codes compared in this study are now in substantial agreement on the processing of ENDF/B-IV evaluated photon production data. Because no format changes in this area are contemplated for ENDF/B-V, the same statement should be true for that data file.

Acknowledgements

The authors wish to acknowledge the constant encouragement and assistance of the Shielding Subcommittee Chairman, Dr. R. W. Roussin and the constructive discussion of Dr. H. Henryson II, of the Applied Physics Division, Argonne National Laboratory. Ms. B. R. Diggs contributed significantly to the ORNL LAPHNGAS calculational effort. Research sponsored by the U. S. Department of Energy.

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