Comparison of Photon-Production Processing Codes
LAPHNGAS, MACK-IV, AND NJOY
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Comparison of Photon-Production Processing Codes

LAPHNGAS, MACK-IV, AND NJOY

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by


ABSTRACT

Several laboratories have independently developed computer codes that 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. Results are tabulated for future comparisons with other codes.

I. 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 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-IV⁵) 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. (The abbreviations used hereinafter for referring to each of the codes are listed in Table I). For the purpose of this report, 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.

<table>
<thead>
<tr>
<th>Code</th>
<th>Laboratory</th>
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<tr>
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<td>Los Alamos</td>
<td>LASL NJOY</td>
</tr>
<tr>
<td>MACK-IV</td>
<td>Argonne</td>
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<tr>
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<td>Los Alamos</td>
<td>LASL LAPH</td>
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</table>

*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.
Section II of this report describes the scope and ground rules of this study. Section III discusses the sources of discrepancies encountered in the course of the study and presents our results and conclusions.

Appendix A contains a discussion of the processing of photon energy spectra in the ENDF/B probability distribution format. Appendix B contains a tabulation of all nonzero matrix elements calculated by the "final versions" of the various codes.

In the following discussions, it is assumed that the reader is familiar with the ENDF terminology described in Ref. 2.

II. METHODOLOGY

The scope of the study, summarized in Table II, was similar to the work of Seamon\(^3\) except for the fact that higher order matrices were calculated for \(^{12}\text{C}\), \(^{14}\text{N}\), and \(^{16}\text{O}\). 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

<table>
<thead>
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<th>ISOTOPES AND REACTIONS CONSIDERED IN THIS STUDY</th>
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<table>
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<th>ENDF/B-IV MAT</th>
<th>MT</th>
<th>MF=12/13</th>
<th>LF(^a)</th>
<th>E(_{\text{INT}}) (^b)</th>
<th>E(_{\text{INT}})</th>
<th>E(_{\text{Y,INT}}) (^b)</th>
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<td>O-16</td>
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<td>TPA</td>
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\(^{a}\)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.
complex cascade of transition probability arrays was processed for $^{23}\text{Na}$. (To illustrate the complexity of the $^{23}\text{Na}$ transition probability data, the MT60 cascade is depicted in Fig. 1.) The neutron and photon energy group structures used in this study are listed in Table III. 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.

**TABLE III**

**GROUP BOUNDARIES IN ELECTRON VOLTS**

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

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 (Table IV) 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 as in Table V. 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 $1.0 \times 10^{-6}$b were similarly disregarded. The choice of NJOY as the standard of comparison was completely arbitrary.

III. RESULTS AND 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
### TABLE IV

**A SAMPLE OF THE SIDE-BY-SIDE LISTING PROVIDED TO EACH PARTICIPANT**

<table>
<thead>
<tr>
<th>NG</th>
<th>PG</th>
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<th>NJOY</th>
<th>LAPHNGAS</th>
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### TABLE V

**A SAMPLE OF THE PERCENTAGE DIFFERENCE LISTING PROVIDED TO EACH PARTICIPANT**

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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 that are expressed in ENDF/B as normalized probability distributions \( g(E_{\gamma} - E_i) \) 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 \( E_i^{++} \); at the higher neutron energy \( E_{i+1} \), the photon endpoint energy becomes \( E_{i+1}^{++} \). 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 \( E_{i+1}^{++} \), whereas the interpolation method used by MACK-IV [Fig. 2(b)] gives photon yields only up to an energy of \( E_i^{++} \). Because the resulting intermediate distributions are normalized, the NJOY/LAPHNGAS method gives more 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 \( E_i^{++} \) and \( E_{i+1}^{++} \). However, the current formats and procedures for ENDF/B-IV do not allow for an interpolation scheme that would produce the physically reasonable result. The fluorine results for MT = 102 show the impact of the different interpolation methods. Appendix A of this report presents a more detailed discussion of this problem and a recommendation for altering the ENDF representation of these data.

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 \( E_{\gamma} \) to be calculated from the target atomic mass ratio AWR and the neutron energy \( E_n \) according to the formula

\*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.

\[ E_{\gamma} = E_{\gamma}^{i} + \frac{AWR}{AWR + 1} \times E_n \]

where \( E_{\gamma}^{i} \) is the discrete photon energy quoted in the ENDF file. The MACK-IV and NJOY codes calculate \( E_{\gamma} \) at each neutron energy within a group, whereas LAPHNGAS calculates one value of \( E_{\gamma} \) using the group-average neutron
energy $E_n$. 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 a linear interpolation scheme 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.

ACKNOWLEDGMENTS

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.

APPENDIX A

PROCESSING OF PHOTON ENERGY SPECTRA IN THE PROBABILITY DISTRIBUTION FORMAT*

Continuous energy distributions of secondary photons, expressed as normalized probability distributions, are given in File 15 of ENDF. The distribution functions, $g(E_{\gamma} + E_i)$, are described in TAB2 format, where different TAB1 records are used to represent $g(E_{\gamma} + E_i)$ at different neutron energies $E_i$.

* A complete description of the formats referred to in this appendix can be found in the ENDF format manual (see Ref. 2).
The TAB1 records within a subsection are given in increasing order of neutron energy, and the photon yields within any TAB1 record are given in increasing order of photon energy $E_\gamma$. The endpoint energy of the photon spectrum increases with neutron energy, which means the TAB1 records span different photon energy ranges. This data representation generates an ambiguous situation for the interpolation between TAB1 records to get the spectrum at neutron energy $E_{i+1}$, between $E_i$ and $E_{i+1}$. The LAPHNGBAS and NJOY codes extend the TAB1 record to perform the interpolation assuming a value of zero for $g(E_\gamma + E_i)$ at photon energies beyond $E_\gamma^i$ [Fig. 2(a)]. This approach overestimates the total photon energy yield and can lead to a negative energy for the recoil nucleus. An alternative approach, used by MACK-IV, is to stop the interpolation process at $E_\gamma^i$ [Fig. 2(b)], thereby underestimating the photon energy yield. This approach leads to an overestimate for the energy of the recoil nucleus.

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. A-1, 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 similar situation exists for secondary neutron spectra in File 5 of ENDF.
A further source of difficulty with the normalized probability distributions is the use of this format to represent discrete photons. Figure A-2 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 calculated at ANL, and the results are tabulated in Table A-I. The maximum difference of 14% in group 4 represents an important discrepancy for many applications. These data demonstrate the difficulties that can result from the use of File 15 to represent discrete photons.

Fig. A-2. Representative normalized probability distribution functions $g(E_y+E_i)$ for fluorine (MAT1277, MT102).
TABLE A-I

PERCENT DIFFERENCE IN GAMMA ENERGY PER NEUTRON GROUP
FOR 19F MAT = 1277, MT = 102

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<sup>a</sup>Percent difference = \(\frac{\text{Overestimate method} - \text{Underestimate method}}{\text{Underestimate method}} \times 100.00\)

APPENDIX B

A LISTING OF THE NONZERO MATRIX ELEMENTS

The listing below is a reproduction of the side-by-side listing of all nonzero matrix elements, as they were calculated by the various codes after all corrections were made to the processing codes. Small differences still exist which were not considered serious enough to pursue. Large differences in higher order matrices are due to the fact that LAPHXGAS matrix elements include a factor of \((2\xi + 1)\) while NJOY results do not.

In the listings below, the abbreviation "NG" refers to the neutron groups and "PG" refers to the photon groups. Group structures are given in Table III.
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### Gamma Production Core - Comparison

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### Gamma Production Core - Comparison

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### Gamma Production Core - Comparison

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### Gamma Production Cone Comparison

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### Gamma Production Cone Comparison

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**GAMMA PRODUCTION CONE - COMPARISON**

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### Gamma Production Cone Comparison

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