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Discrete-energy Gamma-rays from MCNP Data Libraries

Abstract

Lists of discrete gamma-ray lines, induced by neutron reactions, have been produced for several of the neutron transport data libraries. The lines, and relative strengths, from each nuclide are given. These lists can be useful to people modeling the generation of gamma-rays with codes which utilize MCNPTM compatible data libraries. We describe where to obtain files containing such listings, and how to interpret and use the information on them.

I. Introduction

A new set of DISCRETE Energy Gamma-ray (DISCEGAM) files has been produced, to aid MCNP* users who are interested in neutron-induced photons. For each of the most common libraries of nuclear transport data, there is a corresponding DISCEGAM file, listing the discrete gamma-ray lines (as represented in the transport data) that can be generated during neutron transport. Such information may be useful in choosing the best library for an application, in setting up tallies for output photons [1, page 3-75ff], or in biasing the photon source generation with the use of PIKMT cards [1, page 3-100]. With these applications in mind, we use the terms *gamma-ray* and *photon* interchangeably in this Research Note.

In the following section, we show how to obtain a DISCEGAM file, and give an overview of its format. Next, in Section III, we describe the contents of the "Gamma-ray Line List" table, which is the most commonly used table on the DISCEGAM file; and, in Section IV, we discuss the other tables on the file. Finally, in the Conclusion, we point out some general considerations that the users of DISCEGAM data should keep in mind.

II. Overview of DISCEGAM Files

A DISCEGAM file is produced at Los Alamos by running the DEG ("Discrete Energy Gamma") code[2]. This code scans through an MCNP nuclear data library, nuclide by nuclide, and processes all datasets which pertain to incident neutrons, with either continuous-energy or discrete-energy treatment, and which contain "enhanced

*MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory

Library Name	DISCEGAM Filename	Number of Nuclides on Library (Total)	(Photon-Generating)	Total Gamma-ray Lines in Library
rmccs	rmccs.deg	64	54	1287
rmccsa	rmccsa.deg	27	15	236
rmccsb	rmccsb.deg	6	6	86
endf60	endf60.deg	122	84	3461

Table 1: MCNP transport data libraries and corresponding DISCEGAM files.

photon-production” data. (Note that the same photons will be obtained with the discrete-energy data as with the corresponding continuous-energy data.)

Available DISCEGAM Files. Table 1 lists the transport data libraries for which DISCEGAM files have been produced, along with some library-wide statistics in each case. The DISCEGAM files can be located on the World Wide Web under the following:

<http://www-xdiv.lanl.gov/XCI/data/document.html>

The ASCII files are the direct output of the DEG program; they contain page-eject characters (“1”) in column 1, and have lines up to 130 characters long. The PDF files contain images of the ASCII files, written with a small font; they are provided primarily for printing when the ASCII line-width cannot be handled on a printer. For users with access to the Los Alamos CFS file storage system (on both open and secure), there are copies of the DISCEGAM files, and of this memo, under directory: `/x6data/doc/discegam`.

Structure of a DISCEGAM File. Each DISCEGAM file is composed of four parts:

1. The first part is a “Users Guide” to the data tables which follow on the file; its contents are similar to those of this Research Note. With this information, each DISCEGAM file should be mostly self-describing.
2. The second part contains the “Gamma-ray Line List”, showing the discrete neutron-induced photons, sorted by photon energy, for each nuclide on the library which has photon-production data. This nuclide-by-nuclide list is the primary result in DISCEGAM, and is described in detail in Section III below.
3. The third part contains the “Library-Wide Line” tabulation, where all of the photon lines, from all of the nuclides in the library, are combined into one energy-sorted list. See Section IV below.
4. The last part contains a list of “Total Cross Sections”. For each photon-producing nuclide, the “total neutron collision cross section” and “total photon-production cross section” are given. This table is also described in Section IV below.

In each list of cross sections (parts 2 through 4 of the DISCEGAM file), the data are given at three incident neutron “test” energies: 2.53E-8 MeV, 1 MeV, and 14 MeV (the 2.53E-8 MeV neutron energy is labeled “thermal”).

```

-----
Z= 4 beryllium
be- 9
ZAID= 4009.60c
(endf602)
-----

-----
strong photons
-----

n      Egam  p/np  RT      |      cross sections      |      strengths      |      specific intensity      |      source      width
-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----
      |      |      |      |      |      |      |      |      |      |      |      |      |
1  0.47700  n-p  701001 |  0.00E+00  0.00E+00  5.00E-03 |  0.00E+00  0.00E+00  9.16E-01 |  0.00E+00  0.00E+00  1.00E+00 | (n,t)*      |
2  0.85300  np*  102001 |  2.20E-03  2.89E-05  7.25E-05 |  1.58E-01  1.58E-01  1.33E-02 |  2.55E-01  2.89E-01  7.25E-01 | (n,gamma)  +1.000
3  2.59000  np*  102001 |  2.09E-03  2.74E-05  6.88E-05 |  1.50E-01  1.50E-01  1.26E-02 |  2.42E-01  2.74E-01  6.88E-01 | (n,gamma)  +1.000
4  3.36800  np*  102001 |  2.97E-03  3.89E-05  9.79E-05 |  2.14E-01  2.14E-01  1.79E-02 |  3.44E-01  3.89E-01  9.79E-01 | (n,gamma)  +1.000
5  6.81000  np*  102001 |  5.43E-03  7.12E-05  1.79E-04 |  3.91E-01  3.91E-01  3.28E-02 |  6.29E-01  7.12E-01  1.79E+00 | (n,gamma)  +1.000

-----
weak photons
-----

n      Egam  p/np  RT      |      cross sections      |      strengths      |      specific intensity      |      source      width
-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----
      |      |      |      |      |      |      |      |      |      |      |      |      |
1  3.44400  np*  102001 |  1.03E-03  1.35E-05  3.39E-05 |  7.40E-02  7.40E-02  6.20E-03 |  1.19E-01  1.35E-01  3.39E-01 | (n,gamma)  +1.000
2  5.95800  np*  102001 |  1.73E-04  2.26E-06  5.69E-06 |  1.24E-02  1.24E-02  1.04E-03 |  2.00E-02  2.26E-02  5.69E-02 | (n,gamma)  +1.000

```

Figure 1: Gamma-ray Line List for the ${}^9\text{Be}$ isotope in the ENDF60 library. There happen to be 7 discrete gamma-ray lines in the dataset for this isotope — five “strong” and two “weak”.

III. Interpretation of Gamma-ray Line List

A portion of a Gamma-ray Line List is shown in Figure 1. This portion shows the discrete gamma-ray lines induced by neutron collisions with ${}^9\text{Be}$, as represented in the ENDF60 library; the complete list contains similar data for all pertinent isotopes on the library. Each target nuclide is introduced by a header giving the element name and symbol, the “ZAID” of the dataset, and the library file it appears in; in this case, the file “endf602” is a type-2 version of the ENDF60 library.

The data is broken into two parts: “strong photons” and “weak photons”. The former is defined as a line contributing at least 10% of all of the photons produced by neutron reactions on the specific target nuclide, for one or more of the incident neutron “test” energies. For each discrete photon line, the following quantities are given:

n This is just the index, in energy order, of the line.

Egam This is the discrete photon energy, in MeV. Note that there are cases where the same photon transition occurs for more than one “source” (neutron) reaction, such as for the inelastic reactions. In the table, they appear as different photons, but with the same energy, and for many purposes, the user should sum their cross sections (at a given incident neutron energy) to obtain a total production cross section for that particular gamma-ray.

p/np This indicates whether the particular photon is a primary or non-primary photon. The designation “n-p” means a non-primary photon; in this case, the photon energy is always exactly equal to E_{gam} . On the other hand, for a primary photon (designated by

“p”), the energy of the photon produced equals $E_{gam} + \{(awr)/(awr + 1)\} \times E_{neut}$, where awr is the atomic weight ratio (target nuclide mass divided by neutron mass), and E_{neut} is the incident neutron energy. The value of awr may be obtained from Appendix G of the MCNP manual[1] for each nuclide. Primary photons, therefore, are generally useful as signature photons only when produced by thermal neutrons; for this reason, only “thermal” cross section data are listed for such photons. A flag designation of “np*” is used to specify a non-primary photon which has been represented as “almost-but-not-quite-discrete” by the evaluator; that is, it is represented by an isolated, narrow, peak in a continuum spectrum.

MT This is the partial photon-production MT number. For a description of these MT numbers, see the MCNP Manual[1]; the photon production MT numbers are contained in the MTRP Block, described in Table F.6 in Appendix F of the Manual. This MT value can be used on an FM card (page 3–77 of the Manual) as a flux multiplier to determine the number of photons produced with energy E_{gam} , or on a PIKMT card (page 3–100 of the Manual) to bias the photon source. Note that a single photon-production MT can represent a series of output lines, such as in ${}^9\text{Be}$ (Figure 1). When this occurs, all of these lines have the same “MT”, and so the tally or source weighting must be viewed as applying to the neutron reaction (not to the generation of any single photon). This may or may not be what the MCNP user desires.

cross sections These are the photon-production cross sections, in barns, for the individual photon in question (at each of the “test” energies). Note that the listing may contain lines which appear in the photon spectrum, but whose “source” (neutron) reaction cross section happens to be zero at all of the “test” energies; such entries are legitimate, but of limited utility.

strengths These are the relative strengths of the individual photon line for each of the incident neutron “test” energies. Here, strength is defined as the ratio of the individual photon-production cross section to the total photon-production cross section, or, in other words, as the fraction of the total photons produced which have energy E_{gam} , at a given incident neutron energy.

specific intensity This is the photon yield (number of photons generated) in the specified line, for that specific source neutron reaction. It is calculated as the ratio of the individual photon-production cross section to the neutron cross section corresponding to that reaction “MT”. Some “surprises” may occur in the tables in these columns: all zeroes are printed when the source neutron reaction cross section is not explicitly present in the dataset, or, in other cases, a nonzero “yield” can occur even though the source neutron reaction has a zero cross section. (As an example of the latter situation, consider an inelastic scattering reaction involving a particular excited nuclide state that always emits a specific photon; one can view the photon “yield” as always being unity *for that particular reaction*, but, below threshold, the neutron reaction cross section is zero, as is the photon-production cross section which equals the yield times the neutron reaction cross section.)

source reaction This is the type of neutron reaction responsible for the photon. If the label for the reaction is not known, then the neutron-reaction MT number is shown.

width This applies only to “almost-but-not-quite-discrete” photons. It is the full-width, half-max value for the “peak” in the photon spectrum that represents the discrete line. Note that the units for “width” are keV, while the units for E_{gam} are MeV. Also, if a value of “.0000” is shown, it means that the width is less than 0.00005 keV, but, it is still finite. The DEG code ignores photon lines whose “width” exceeds some specified value; the default DISCEGAM files list only those lines with a “width” less than 10 keV. (This, and other run-specific parameters, are listed near the end of the “Users Guide” section of each DISCEGAM file.)

The MCNP user should keep in mind that photons can be generated anywhere within the distribution peak, when deciding on tally bins. The “width” value is preceded by a “shape flag”: a blank indicates that the bin has a “histogram” shape (E_{gam} is the bin midpoint); a “+” sign signifies a peak in a continuous distribution (with the “width” extending halfway to the neighboring points on each side of the peak); and, a “~” flag signifies that both continuous and histogram binning occurs (in spectra at different incident neutron energies).

IV. Other Information on DISCEGAM Files

There are two “auxiliary” tables on the DISCEGAM file, which, in combination with the main “Gamma-ray Line List”, are useful in certain applications.

Library-Wide Line Tabulation. When deciding on a signature photon on which to tally, this table is helpful in determining if there is likely to be interference from another nearby (in energy) discrete photon from the same or another isotope in the system. Figure 2 shows an example of this table, taken from the DISCEGAM file for the ENDF60 library.

All of the lines, from all of the isotopes in the library, are listed here, in order of increasing photon energy. For each photon, most of the quantities from the “Gamma-ray Line List” are reproduced; other quantities, such as “specific intensities”, are less useful here, but can be found in the “Gamma-ray Line List”. The target nuclide responsible for each line is described by the symbols in the “isotope”, “ZAID”, and “library” columns; this simplifies cross-comparisons between libraries. The lines are categorized as “weak” or “strong” as in the “Gamma-ray Line List”, but, of course, each cross section needs to be weighted by the appropriate nuclide number density, when comparing line strengths in a mixture.

Table of Total Cross Sections. This list has one line per nuclide, giving the total neutron cross section and the total photon-production cross section at each of the “test” energies. A (partial) example of a “Total Cross Section List” is shown in Figure 3, taken from the DISCEGAM file for the ENDF60 library. The list is useful for “ballpark estimates” of how important an isotope is as a “photon producer”. Note that the ratio of the total photon-production cross section to the total neutron collision cross section is equal to the average number of photons produced, per neutron collision at that incident neutron energy.

DISCEGAM file:"endf60.deg" for data library:"endf602" [deg (mod 4.4) 09/26/97 23:03:17]

LIBRARY-WIDE LINE LIST (energy-ordered)

Order of Strong Photons

isotope	ZAID	Egam	p/np	MT	Cross Sections			Strengths			width (keV)	data library
					thermal	1 MeV	14 MeV	thermal	1 MeV	14 MeV		
ta-181	73181.60c	0.01000	n-p	3027	0.00E+00	1.05E+00	1.51E+00	0.00E+00	2.19E-01	1.38E-01		endf602
fe- 57	26057.60c	0.01400	n-p	51001	0.00E+00	3.95E-01	9.50E-04	0.00E+00	2.23E-01	3.10E-04		endf602
fe- 57	26057.60c	0.01400	n-p	52003	0.00E+00	2.68E-01	1.14E-03	0.00E+00	1.52E-01	3.72E-04		endf602
fe- 57	26057.60c	0.01400	n-p	53006	0.00E+00	2.36E-01	8.01E-04	0.00E+00	1.34E-01	2.61E-04		endf602
.												
o- 16	8016.60c	7.11685	n-p	4002	0.00E+00	0.00E+00	6.54E-02	0.00E+00	0.00E+00	1.02E-01		endf602
li- 6	3006.60c	7.25000	p	102001	2.35E-02			4.39E-01				endf602
pb-207	82207.60c	7.37605	np*	102001	7.13E-01	0.00E+00	0.00E+00	1.00E+00	0.00E+00	0.00E+00	.1000	endf602
al- 27	13027.60c	7.72600	p	102001	6.97E-02			1.47E-01				endf602

order of weak photons

isotope	ZAID	Egam	p/np	MT	Cross Sections			Strengths			width (keV)	data library
					thermal	1 MeV	14 MeV	thermal	1 MeV	14 MeV		
v-nat	23000.60c	0.00200	np*	3073	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	+1.000	endf602
pu-239	94239.60c	0.00785	n-p	4010	0.00E+00	1.42E+00	0.00E+00	0.00E+00	7.61E-02	0.00E+00		endf602
i-127	53127.60c	0.00800	n-p	608001	0.00E+00	0.00E+00	2.69E-05	0.00E+00	0.00E+00	4.34E-06		endf602
i-127	53127.60c	0.00800	n-p	617001	0.00E+00	0.00E+00	1.43E-06	0.00E+00	0.00E+00	2.31E-07		endf602
.												
si-nat	14000.60c	10.61100	p	102001	4.61E-04			1.30E-03				endf602
n- 14	7014.60c	10.83332	p	102001	9.98E-03			6.14E-02				endf602
n- 14	7014.60c	11.05000	n-p	4001	0.00E+00	0.00E+00	4.95E-07	0.00E+00	0.00E+00	1.08E-06		endf602
b- 10	5010.60c	11.45600	p	102001	3.00E-02			8.34E-06				endf602

Figure 2: Example of Library-Wide Line tabulation. Refer to Sections III and IV for explanations of the data in each column.

DISCEGAM file:"endf60.deg" for data library:"endf602" [deg (mod 4.4) 09/26/97 23:03:17]

TOTAL CROSS-SECTIONS (by isotopes)

Cross Section Tabulation

isotope	ZAID	Total neutron cross section			Total photon-production cross section			data library
		thermal	1 MeV	14 MeV	thermal	1 MeV	14 MeV	
h- 1	1001.60c	3.0661E+01	4.2587E+00	6.8903E-01	3.3292E-01	3.4460E-05	2.9830E-05	endf602
h- 2	1002.60c	4.2534E+00	2.8703E+00	8.1001E-01	5.0579E-04	5.7682E-06	9.5000E-06	endf602
li- 6	3006.60c	9.4245E+02	1.2707E+00	1.4490E+00	5.3556E-02	1.6066E-05	1.6141E-03	endf602
li- 7	3007.60c	1.0867E+00	1.5545E+00	1.4417E+00	4.9978E-02	1.8091E-01	6.6895E-02	endf602
.								
cm-248	96248.60c	8.6836E+00	7.5691E+00	6.5803E+00	1.1114E+01	1.9686E+01	2.3647E+01	endf602
cf-250	98250.60c	1.6218E+03	8.4896E+00	5.8930E+00	7.4330E+03	2.2157E+01	2.2841E+01	endf602
cf-251	98251.60c	8.2031E+03	7.9443E+00	5.7643E+00	5.9521E+04	1.7116E+01	2.1944E+01	endf602
cf-252	98252.60c	6.3946E+01	8.3850E+00	5.7508E+00	3.5200E+02	2.0710E+01	2.2868E+01	endf602

Figure 3: Example of Total Cross Section tabulation, for the ENDF60 library.

V. Conclusion

This Research Note has described the DISCEGAM files, which are designed to aid in the modeling or interpretation of systems where the generation of discrete gamma-ray lines is important. However, users must keep in mind some limitations concerning the data in the DISCEGAM files:

- The tables describe the actual data for a given library, not necessarily the reality of nature. Even when an evaluation includes photon-production data, it may have been designed with other applications in mind, or contain only a token set of discrete lines. A previous report[3] contains plots of the combined continuum-plus-discrete photon spectra for nuclides in the main MCNP data libraries, and is an alternative starting point for judging the suitability of the nuclear data for a particular application.
- The nuclides listed in a DISCEGAM file form an incomplete set. Many isotopes are not included in a given library at all, and others don't show up in the tables because they have no photon-production data. Of course, the table listing "all lines" is similarly incomplete.
- Remember that there are neutron-induced photons which do not appear as discrete lines. Depending on the application and the isotope, these "continuum" photons can be as important, or more important, than discrete photons.
- There are options to the DEG code, which affect the recognition of "nearly-discrete lines" embedded in spectral data, and there are also options limiting the search to only spectra generated at the neutron "test energies". The contents of the tables will be (slightly) dependent on these options; for most applications, though, the default DISCEGAM files should be appropriate.

REFERENCES

- [1] J. F. Briesmeister, Editor, "MCNP — A General Monte Carlo N-Particle Transport Code," Los Alamos National Laboratory Report LA-12625-M, Version 4B (UC 705 and UC 700) (March 1997).
- [2] J. C. Comly, "DEG — A Code for Generating DISCEGAM Files," Los Alamos National Laboratory Memo, XCI:97-18(U) (October 1997).
- [3] S. C. Frankle, "Photon Production Assessment for the MCNP Data Libraries," Los Alamos National Laboratory Report LA-13092-MS (UC 700) (March 1996).