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Title: MCNP Delayed-Particle Library – Release 5

Author(s): Wilcox, Trevor
Mckinney, Gregg Walter

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MCNP Delayed-Particle Library – Release 5

T. A. Wilcox and G. W. McKinney

Los Alamos National Laboratory, Bikini Atoll Rd. P.O. Box 1663, MS-C921, Los Alamos, NM 87545
wilcox@lanl.gov, gwm@lanl.gov

INTRODUCTION

Development of a delayed-particle production physics package began in 2004, due to the user communities' desire to have delayed-particle production in MCNP [1]. To support this effort, a data library was created that contained bin-wise delayed neutron data. This was Release 1 of the delayed library (delay_library_v1.dat) which was released with MCNPX 2.6.0 [2].

Release 2 of the delayed library [1] was released with the initial release of MCNP6 (MCNP6 is the merger of MCNPX and MCNP5) [3]. This library included bin-wise data for delayed betas, gammas, and neutrons. Release 3 of the delayed library was never publicly released. Delayed-alpha production was added to Release 4 of the delayed library and was released with MCNP6.1.1 [4].

Release 5 of the delayed library (delay_library_v4.dat) for MCNP has been created from the ENDF/B-VII.1 decay data [5]. The delayed-library file contains data for delayed gammas, neutrons, betas, and alphas. The gamma bin structure has been increase from 25 energy bins to 500 bin, increasing energy spectrum resolution that will be shown later in the paper.

The previous release (Release 4) of the delayed library contained 2611 nuclides with delayed gammas, 279 nuclides with delayed neutrons, 1201 nuclides with delayed betas, and 171 nuclides with delayed alphas. Release 5 of the library contains 1865 nuclides with delayed gammas, 298 nuclides with delayed neutrons, 1891 nuclides with delayed betas, and 248 nuclides with delayed alphas.

The ending energy bin for the gammas data is 10 MeV with 500 equally-spaced bins. There are 750 equally-spaced energy bins for neutrons with the last energy bin being 7.5 MeV. Betas and alphas each have 100 equally-spaced energy bins with the last energy bin at 10 MeV.

DESCRIPTION OF THE ACTUAL WORK

The ENDF2CINDER code has been written to process the raw ENDF tapes. The code reads in the ENDF decay sublibrary and processes file 1 and file 8 data formats [6] into the cindergl.dat and delay_library.dat format. File 1 of the ENDF decay data sublibrary consists of "General Information" about the data. File 8 contains radioactive decay and fission product yield data. In the ENDF decay file gamma and x-ray data are separate entries. In creating the gamma entries in the delayed library the gamma and x-ray data have been combined.

All of the continuum data in the decay file has the interpolation flag E_{int} set to 1. For one dimensional interpolation, E_{int} set to one indicates that a constant histogram approach shall be used [5]. This means that the function is constant and is equal to the value of the function at the lower limit of the bin.

The β-ray spectrum are often given as an endpoint energy and it is up to the user to create the spectrum data. For example, the β-ray spectrum for radium E (Bi-210) is given as the endpoint energy of 1.1621E+06 eV in the ENDF/B-VII.1 decay file. Using the methods described in [7, 8] the energy spectrum can be recreated and is shown in Figure 1. This reconstruction compares with the endpoint energy of 1.17 MeV and a maximum around 150 keV given in [7]. The reader is encouraged to review [8] for a discussion on how to reproduce the spectral curve from the endpoint energy as it is beyond the scope of this paper.

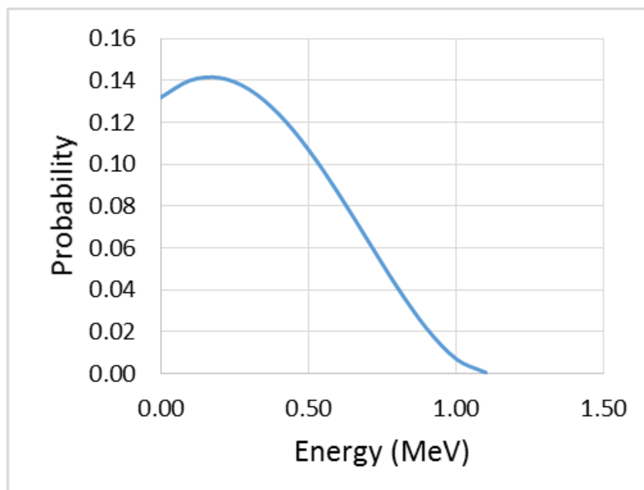

Fig. 1. β-ray Energy Spectrum for Radium E

RESULTS

To use the delayed feature the user needs to have an ACT card and set DG=mg to sample multi-bin delayed gamma data from the delayed library [3]. To sample multi-bin delayed neutrons set DN=model on the ACT card. If the delayed-library file is missing, the code will use the cinder.dat 25-bin gamma data for gamma emission and other delayed particles will not be produced.

Figure 2 gives the delayed gammas emitted from Co-60. The dashed blue line represents the gammas emitted using the previous delayed library (Release 4), while the solid black line is from the new library (Release 5).

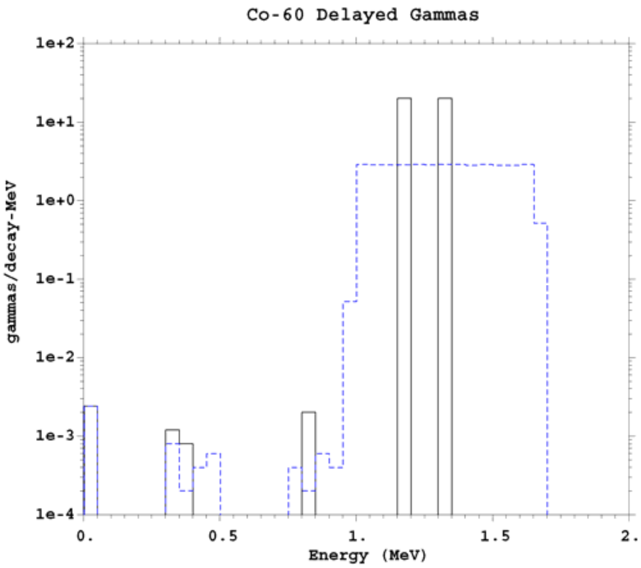

Fig. 2. Delayed Gamma Spectrum from Co-60

By increasing the number of gamma energy bins from 25 to 500, it can been seen in Figure 2 that there is a significant increase in spectrum resolution. The strong gamma lines at 1.17 MeV and 1.33 MeV, which were previously smeared, are now distinguishable using the Release 5 data.

Figure 3 shows the delayed-gamma spectrum from thermal neutron induced fission of U-235. The dashed blue curve is the spectrum from the old library, while the solid black curve is from the new library. As stated previously, the new library has more bin structure for the gamma emission as compared to the old library. The delayed-gamma integral for both libraries is 7.8 γ/f.

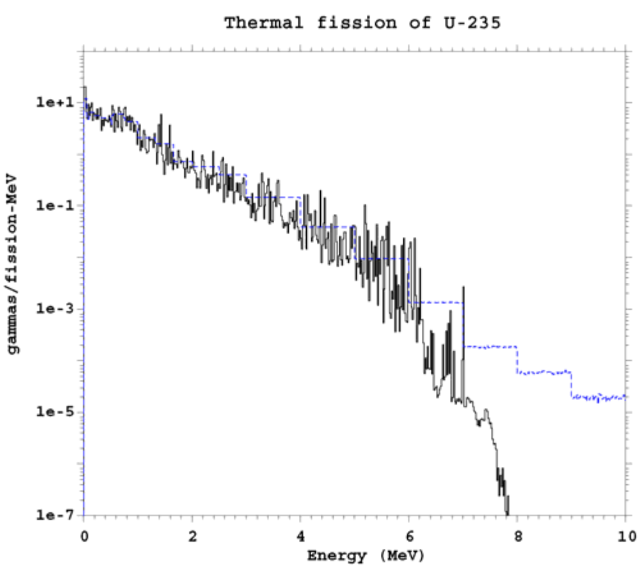

Fig. 3. Delayed Gammas per Thermal Fission

Figure 4 provides the delayed-neutron spectrum from thermal neutron induced fission of U-235. The dashed blue curve is the spectrum from the old library while the solid black curve is from the new library. The delayed-neutron integral for both libraries is 0.019 n/f.

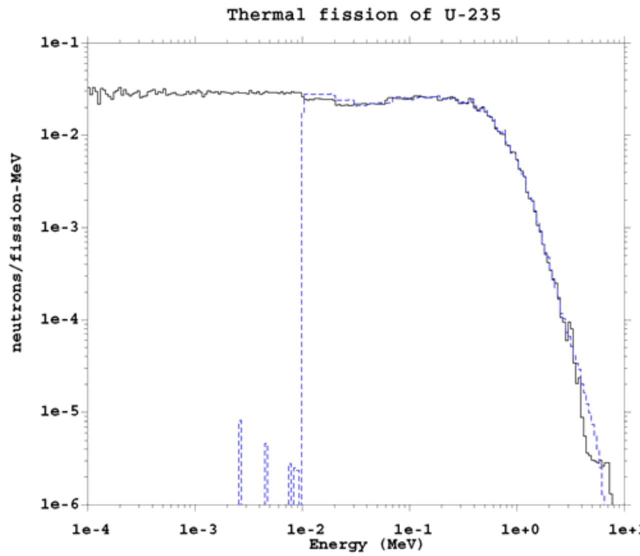

Fig. 4. Delayed Neutrons per Thermal Fission

It should be noted that DN=library on the ACT card means the delayed-neutron data comes from the ACE library, while DN=model means the Cinder routine [9] gets the fission-product distributions from the cinder.dat data file and the delayed neutrons from these fission products comes from delay_library.dat data file.

Figure 5 gives the gammas per decay for the U-238 equilibrium case. The dashed blue curve is Release 4 data and the black solid curve is Release 5 data. The integral number of gammas per decay for the former is 2.26, with 2.33 for the latter. While there is not a significant difference in the integral number of gammas per decay, there is a major difference in the structure of the spectrum. Again, Release 5 has 500 energy bins for gammas, while Release 4 had 25.

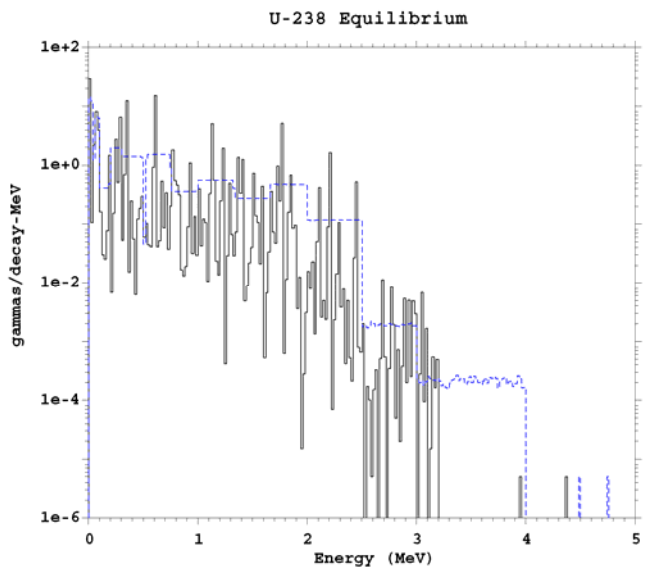

Fig. 5. Delayed Gammas from U-238

Figure 6 shows the betas per decay for the U-238 equilibrium case. The dashed blue curve is Release 4 data and the black solid curve is Release 5 data. The integral number of betas per decay for the former is 3.46, with 9.12 for the latter. For this case, there is a significant difference (a factor of 2.6) in the integral number of betas per decay. This can be seen by the divergence of the two curves between 0 and 2 MeV. The energy bin structures are the same for Release 4 and 5 with 100 bins.

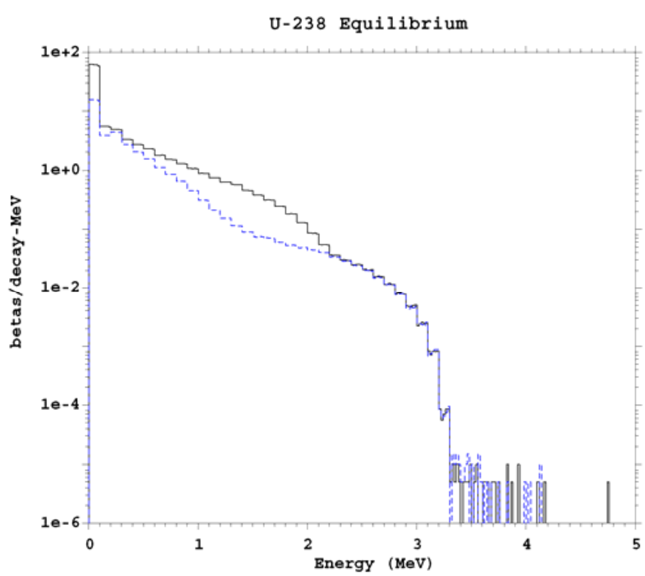

Fig. 6. Delayed Betas from U-238

Figure 7 provides the alphas per decay for the U-238 equilibrium case. It should be noted that most of the dashed blue curve (Release 4 data) lies on the black solid curve (Release 5 data). The integral number of alphas per decay is 6.41 for both releases. The energy-bin structures are the same for Release 4 and 5 with 100 bins.

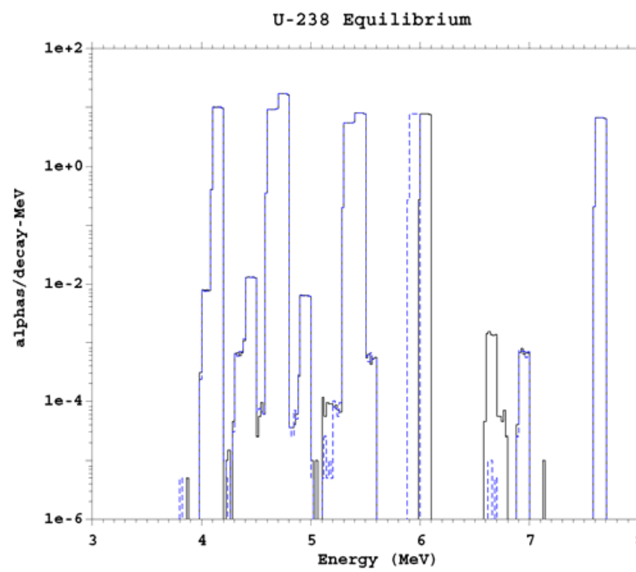

Fig. 7. Delayed Alphas from U-238

CONCLUSION

The delayed library used by MCNP to generated delayed gammas, neutron, betas, and alphas using a multi-bin structure has been updated to ENDF/B-VII.1 decay data. The bin structure for neutrons, betas, and alphas have been preserved from the previous release of the library, while the number of delayed-gamma energy bins have been increased from 25 to 500.

By increasing the number of gamma bins, there is a corresponding increase in the resolution in the results. As the number of bins increase further, the resolution of single line data will be reached, but at a computation cost. Further investigation is required to understand the relationship of the number of bins to the computation time. Once this is understood, a compromise can be reached where the number of bins are maximized while still keeping run times reasonable.

Benchmarking of the new delayed particle data will continue to quantify the accuracy of the ENDF/B-VII.1 decay data and the MCNP algorithms. In addition, the feasibility of incorporating the ability of MCNP to directly read the ENDF decay tape will be researched.

ACKNOWLEDGMENTS

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