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MCNP 6.2.0 Delayed-Particle Production Improvements

J. R. Tutt, G. W. McKinney, T. A. Wilcox, and G. E. McMath

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

I. INTRODUCTION

Development began on a delayed-particle physics package for the Monte Carlo Radiation transport code MCNPX in 2004 incorporating the CINDER90 depletion code and delayed particle libraries. When MCNP5 was merged with MCNPX to form MCNP6 [1] in 2010, this delayed-particle capability was passed on and has been continuously improved in subsequent versions of MCNP6 [2]. Today, the delayed-particle feature in MCNP6 allows for the production of delayed neutrons, gammas, betas, and alpha particles [3]. Future development includes the addition of delayed-positron production in the next release of MCNP6.

Delayed particles can be sampled with MCNP using the ACT card in conjunction with the FISSION and NONFISS keywords. The user can specify one or more of the four available delayed-particle types mentioned above on one or both of the FISSION and NONFISS keywords. If a delayed-particle type is selected on the FISSION keyword, then delayed production of that particle from fission products and their progeny will be produced. Likewise, if a delayed-particle type is selected on the NONFISS keyword then delayed production of that particle from non-fission interactions and spontaneous decay will be produced [1]. In some cases, the sheer number of delayed particles that can be produced from nuclear reactions and spontaneous decay (i.e. hundreds of delayed gamma lines when spontaneous fission is possible) can make it difficult to achieve converged solutions in an efficient and timely manner. Truncation methods are the simplest form of variance reduction and can be used to decrease convergence times by limiting calculations to the phase space of interest [4]. This paper introduces several such truncation methods that allow the user to restrict the number of possible delayed particles available for sampling to only those of interest in the problem. It is important to stress that the use of any truncation method should be verified by first assessing the impact of the truncated particles (i.e. by disabling the truncation) for one or more baseline cases. In addition to these new methods, a new delayed-gamma sampling algorithm implemented in MCNP 6.2.0 is introduced. Comparisons to ENDF data and analytical benchmarking with the new algorithm show a substantial improvement in accuracy over previous versions.

II. DESCRIPTION OF ACTUAL WORK

II.A. Updated THRESH Usage

Some radionuclides and their daughters exhibit a large number of possible delayed particles, particularly delayed-gamma and x-ray lines, associated with their decay chain. This fact is readily apparent in the lengthy decay chains of actinides which are commonly modeled by the MCNP community. Storing and sampling from the emission data of each discrete particle line for each daughter in a decay chain is memory intensive and requires a large number of histories to suitably converge low amplitude delayed-particle emission lines. For this reason, the THRESH option on the ACT card was introduced in previous versions of MCNP to control the fraction of highest-amplitude discrete delayed-gamma lines that are sampled in a particular problem [1]. By default, the value of THRESH is set to 0.95 and therefor those lines with an amplitude less than 5% of the highest-amplitude delayed-particle line are truncated. When first implemented, the truncation of delayed-particle lines was done on a nuclide-by-nuclide basis during initialization. In other words, the fraction specified on the THRESH keyword was applied to the highest amplitude delayed-gamma line for each individual radionuclide. Lines that fell below 5% of the highest amplitude line would be truncated separately for each individual radionuclide in a given decay chain. Since the threshold value under which lines were truncated was dependent on the highest-amplitude delayed-gamma line for each individual radionuclide, this method caused the truncation of delayed-particle lines to be applied unevenly across decay chains, allowing some low-amplitude lines to escape filtering. In response to this issue, a new treatment has been implemented in MCNP 6.2.0 for the truncation of lines with the THRESH keyword. Rather than applying the specified fraction individually to each radionuclide in a decay chain, line truncation is handled during source sampling and applied to all delayed-particle lines in a chain equally with regard only to the highest-amplitude delayed-gamma line in that chain. This method ensures that low amplitude lines are truncated correctly across the entire decay chain and independently of the emitting nuclei. If the user requires a larger percentage of delayed-gamma lines to be sampled the value of THRESH can be increased accordingly. Setting the value of THRESH to 1 will retain all delayed-particle lines for sampling, however, this may cause some problems to run slowly or exceed memory limits and fail [1]. Fig. 1 shows a comparison between the new and old THRESH usage.

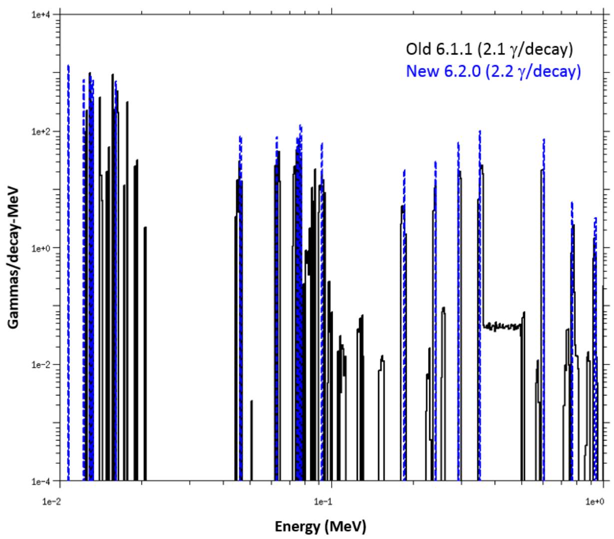

Fig. 1. Comparison of delayed-gamma spectrum from spontaneous decay of U-238 between old THRESH usage in MCNP 6.1.1 (black) and new usage in MCNP 6.2.0 (blue). Note that lower amplitude lines are retained in the old version. Difference in peak height is caused by artificial broadening of the old delayed-gamma algorithm (discussed in II.D).

II.B. Photon Energy Cutoff

In many cases, radionuclides emit a significant number of lower energy delayed-gamma and x-ray lines. The multitude of such lines requires a large number of histories to sufficiently converge solutions. In applications where these low energy gammas are not relevant, tally statistics can be improved, and therefore run time reduced, through the expunging of low energy gamma/x-ray lines that are not of interest (e.g., photon detector modeling, shielded photon sources). The PECUT keyword has been added to the ACT card to allow the user to truncate delayed gamma lines below a specified energy threshold. The value of PECUT is defined in MeV and has a value of 0 by default. By reassigning this value, the user can define a photon energy cutoff under which delayed-gamma/x-ray lines are eliminated from sampling. Fig. 2 shows a comparison of the decay spectrum for a bare sphere made up of the uranium isotopes 233, 234, 235, 236, and 238. In both cases, the value of THRESH was set to 0.99 while the PECUT feature was left at 0 in the black data set and set to 0.1 in the blue data set. The resulting plot shows photon emission lines below 0.1 MeV are omitted from sampling, and delayed particle production only occurs above that limit.

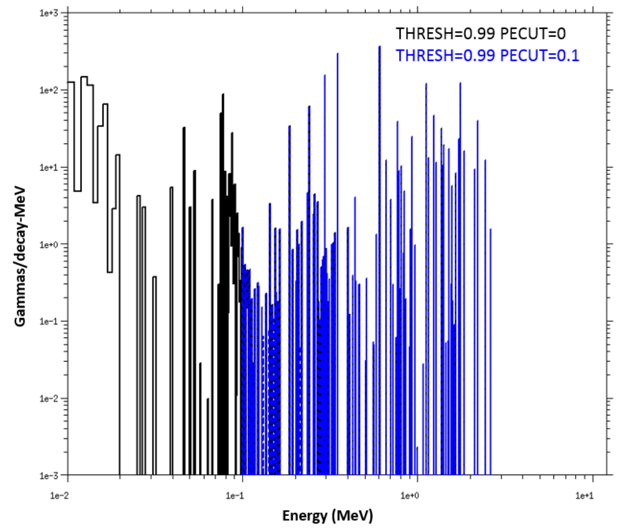

Fig. 2. Delayed-gamma spectrum from uranium Godiva material with (blue) and without (black) PECUT option. Note delayed-gamma production below 0.1 MeV is omitted when PECUT=0.1.

II.C. Spontaneous Decay Half-life Cutoff

Similar to the THRESH and PECUT options, the HLCUT keyword has been added to the ACT card to allow the user further control of spontaneous decay sampling in a given decay chain. Invoking the HLCUT keyword allows the user to set a half-life (in seconds) threshold above which delayed-particle production from this and subsequent daughters is truncated. This feature can be used to limit the number of nuclides from which delayed particles are sampled and is useful when lengthy decay chains are involved or a particular subset of a decay chain is to be examined. Fig. 3 shows a spectrum from the same bare uranium sphere as described in section II.B, this time with HLCUT set to 1×10^{11} seconds (blue curve). This eliminates sampling from radionuclides in the various uranium decay chains as follows:

$\mathbf{^{233}U} \rightarrow {}^{229}Th$
$\mathbf{^{234}U} \rightarrow {}^{230}Th$
$\mathbf{^{235}U} \rightarrow \mathbf{^{231}Th} \rightarrow {}^{231}Pa$
$\mathbf{^{236}U} \rightarrow {}^{232}Th$
$\mathbf{^{238}U} \rightarrow \mathbf{^{234}Th} \rightarrow \mathbf{^{234}Pa} \rightarrow {}^{234}U$

where delayed-particle production is included for only the radionuclides in bold, along with production from decay chains related to spontaneous fission. The result is a significant reduction in the number of photon emission-lines that are sampled.

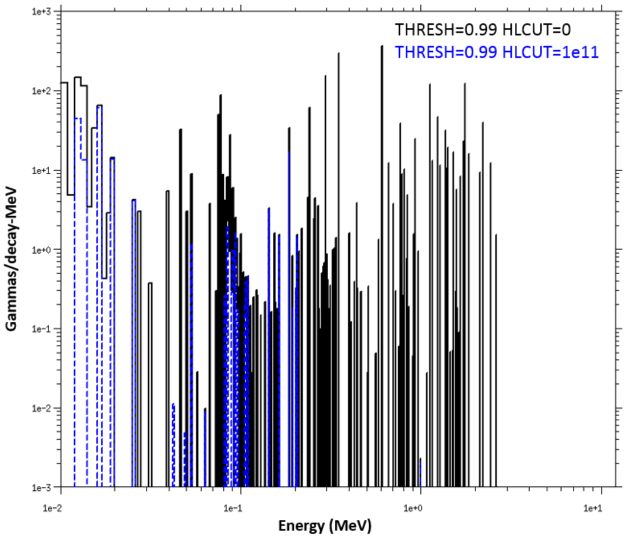

Fig. 3. Delayed-gamma spectrum from uranium Godiva material with (blue) and without (black) HLCUT option. Note the number of delayed-gamma lines is significantly reduced when HLCUT=1e11 is invoked.

II.D. Delayed-Gamma Exact Energy Sampling

In previous versions of MCNP, the delayed-gamma sampling algorithm stored emission-line data from the cindergl.dat data file in a refined energy bin structure. When a line was sampled, the corresponding refined bin was selected and a random energy chosen within that bin. This energy was then applied to the original emission line data to sample the closest line. This method led to biased sampling of low amplitude emission lines near a prominent peak. To address this oversampling of low amplitude delayed-gamma lines, a new method for sampling from delayed-gamma emission data has been implemented. Rather than storing emission data in a refined-bin structure, delayed-gamma emission data is stored in a line-by-line cumulative distribution function (CDF) from which line emissions are sampled directly. The result is exact sampling of delayed-gamma lines. The significant improvement of this CDF sampling method over the old bin method can be seen in Fig. 4 and Fig. 5 which show a U-238 spontaneous decay spectrum from MCNP (black lines) compared directly to ENDF B-VII.1 data (blue points shaded to represent emitting nuclide). Although remarkable agreement is shown in Fig. 5, several discrepancies do still appear between the ENDF and MCNP tally lines that should be explained. First, the MCNP data was tallied in linearly-spaced energy bins and is presented here on a log-log scale which is responsible for the slight left shift in the points between 10 and 100 keV and poor resolution of these low-energy lines. Another discrepancy occurs where the amplitude of a line appears higher (see prominent Th-234 line around 100 keV). This is a result of two or more lines occurring in such close proximity that they are tallied together into one single energy bin resulting in the peak height being a summation line amplitudes.

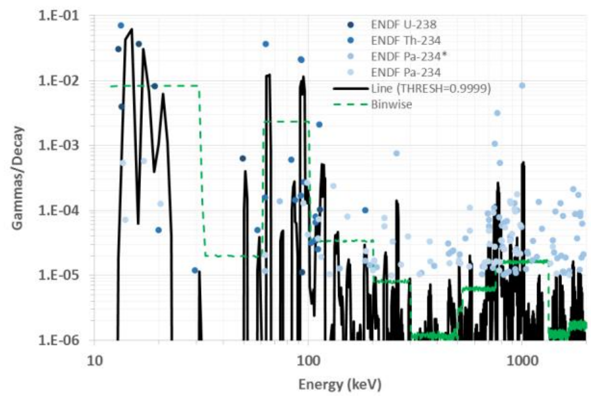

Fig. 4. U-238 spontaneous decay tallies from MCNP 6.1.1 using the refined-bin structure delayed-gamma sampling algorithm compared directly to ENDF B-IIV.1 decay data. There is a distinct broadening effect and line amplitudes do not agree with ENDF data.

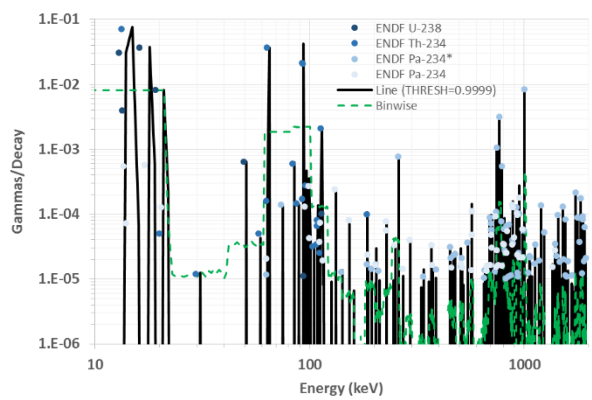

Fig. 5. U-238 spontaneous decay tallies from MCNP 6.2.0 using the new exact energy delayed-gamma sampling algorithm compared directly to ENDF B-IIV.1 decay data. Each line is discrete and has an amplitude that agrees with ENDF data.

The addition of exact line sampling for delayed gammas versus the previous refined-bin structure has improved the agreement of MCNP to analytic spontaneous decay equations. In a paper by R.A. Weldon et al. [5], the delayed gamma capability in MCNP 6.1.1 was benchmarked to closed-form analytic solutions of the Bateman equation for particular decay chains. Results from that paper have been reproduced here in Table 1. This benchmark was repeated with the upgraded sampling algorithm implemented in MCNP 6.2.0. The results of this new benchmark are reported in percent difference in Table 2 and show a significant improvement in agreement between MCNP and analytic calculations.

TABLE 1. MCNP 6.1.1 Analytic Benchmark Results

Radionuclide	Lines (MeV)	1 min	1 hr	1 day	1 yr	100 yr
Mg-28	0.031	2.8%	2.9%	2.8%	2.8%	2.8%
	0.401	4.5%	2.9%	2.8%	2.8%	2.8%
	0.941	0.9%	2.7%	2.8%	2.9%	2.9%
	1.342	2.5%	2.8%	2.9%	2.9%	2.9%
	1.373	0.2%	3.2%	2.8%	2.8%	2.8%
	1.589	2.3%	3.1%	2.6%	2.8%	2.8%
Al-28	1.779	-41.2%	-39.5%	-39.4%	-37.6%	-37.6%
Ar-42	0.000	NA	NA	NA	NA	NA
K-42	1.525			-55.6%	-57.4%	-56.9%
Cs-137	0.000	NA	NA	NA	NA	NA
Ba-137	0.662		-0.6%	-5.8%	-5.3%	-4.0%
Fe-60	0.000	NA	NA	NA	NA	NA
Co-60	1.173					-56.0%
	1.333					-53.7%
Ca-47	0.489	1.9%	4.1%	4.4%	4.4%	4.4%
	0.808	9.4%	4.9%	4.6%	4.5%	4.5%
	1.297	2.6%	4.2%	4.4%	4.4%	4.4%
Sc-47	0.159		0.4%	0.1%	4.6%	4.6%

TABLE 2. MCNP 6.2.0 Analytic Benchmark Results

Radionuclide	Lines (MeV)	1 min	1 hr	1 day	1 yr	100 yr
Mg-28	0.031	-0.2%	0.0%	0.0%	2.8%	2.8%
	0.401	0.3%	0.0%	0.0%	2.8%	2.8%
	0.941	0.2%	-0.1%	0.0%	2.9%	2.9%
	1.342	0.1%	-0.1%	0.0%	2.8%	2.8%
	1.373	-0.2%	0.3%	0.0%	2.8%	2.8%
	1.589	1.3%	0.1%	0.1%	2.9%	2.9%
Al-28	1.779	0.1%	-0.1%	0.0%	2.9%	2.9%
Ar-42	0.000	NA	NA	NA	NA	NA
K-42	1.525			1.7%	0.0%	1.3%
Cs-137	0.000	NA	NA	NA	NA	NA
Ba-137	0.662		-2.0%	-4.8%	-5.4%	-4.0%
Fe-60	0.000	NA	NA	NA	NA	NA
Co-60	1.173					-1.3%
	1.333					0.3%
Ca-47	0.489	0.2%	0.0%	0.0%	4.4%	4.4%
	0.808	0.0%	-0.1%	-0.1%	4.4%	4.4%
	1.297	0.1%	0.0%	0.0%	4.4%	4.4%
Sc-47	0.159		1.9%	0.3%	4.6%	4.6%

III. CONCLUSIONS

New improvements to the delayed-particle capability have been added to MCNP 6.2.0. These improvements include an updated treatment of the THRESH keyword which omits delayed-particle lines below a set amplitude, and addition of the PECUT and HLCUT keywords which allow the user to truncate delayed-particles lines based on energy and half-life, respectively. The delayed-gamma sampling algorithm has also been improved to allow exact energy sampling. Comparisons of MCNP calculations directly to ENDF data and analytical benchmarks have verified the significant improvement in the new delayed-gamma sampling algorithm.

IV. ACKNOWLEDGEMENTS

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V. REFERENCES

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