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Delayed-Gamma Energy Biasing with Exact Energy Sampling in MCNP 6.2.0

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INTRODUCTION

Characterization of delayed-particle signatures is of the utmost importance for detecting, identifying, and quantifying special nuclear material (SNM). Various non-destructive assay (NDA) techniques used in nuclear material safeguards rely on characteristic gamma-ray or neutron emissions to infer properties of a material. The all-particle, all-energy Monte-Carlo radiation transport code MCNP6 [1] is capable of simulating delayed-particle signatures from SNM in addition to modeling the transport of emitted particles to a detector or other instrument.

In some cases, NDA techniques require the measurement of low probability emissions from a given material. In physical scenarios this problem can be bypassed by longer count-times or may be simply irrelevant due to the mass, and therefore the total activity, of the material being measured. However, when applying the Monte-Carlo method to such scenarios, sampling of low probability emissions requires a large number of histories to converge to a statistically acceptable solution. To address this issue, the delayed-neutron and gamma energy biasing feature was introduced in MCNP6 by H. Armstrong et al. [2] in 2013 which allows the user to set up energy windows in which delayed-particle emission sampling can be adjusted. For delayed-gamma sampling, this biasing method was based on the bin-wise structure of gamma emission data for both the multi-bin gamma and line-emission sampling modes.

Recent improvements have been made to the line-emission sampling algorithm which upgrade the previous mini-bin sampling treatment to an exact energy-line treatment [3]. This upgrade was not compatible with the biasing method implemented by H. Armstrong et al. due to the sampled data no longer having a bin-wise structure in line-emission mode. For this reason the delayed-gamma energy biasing feature has been rewritten to support the exact line-sampling treatment.

This paper provides a description of the delayed-gamma energy biasing (DGEB) feature in MCNP6 as well as results and discussion for a gamma-ray spectroscopy example used to demonstrate the biasing utility.

DELAYED-GAMMAS AND ENERGY BIASING

Two modes exist for sampling delayed-photon data in MCNP6; (1) multi-bin gamma sampling mode (DG=MG) in which delayed-gammas are sampled from 500 energy bin-wise data in delay_libraray_v5.dat (available for 1865 nuclides), and (2) line-emission sampling mode (DG=LINE) which samples exact energy line data from ENDF/B-VII contained in cindergl.dat (available for 3475 nuclides and supplemented by multi-bin data). Multi-bin gamma sampling is computationally faster than line-emission gamma sampling and is preferred when high spectral resolution is not required (ex. dose calculations). However, line-emission sampling provides higher fidelity for applications in which individual line-amplitude detail is required (ex. spectroscopy) at the cost of higher computing and memory loads. The delayed-gamma sampling mode is chosen on the activation control (ACT) card through the delayed-gamma data source (DG) keyword. Fig. 1 shows a comparison of the gamma emission spectra between 0.1 and 0.3 MeV from natural uranium using both the line-emission and multi-bin gamma sampling modes.

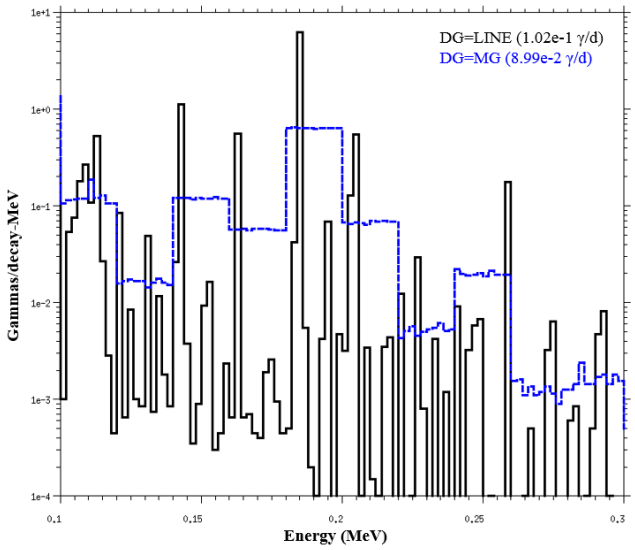

Fig. 1 – Gamma emission spectrum from natural uranium for 0.1 to 0.3 MeV. Integral values are provided in parenthesis.

The delayed-gamma energy biasing feature is accessed through the DGEB keyword on the ACT card and takes the form:

$$\text{DGEB} = w_1, e_1, w_2, e_2, \cdots w_n, e_n$$

where w_m is the weight for the m^{th} energy bin and e_m is the upper energy bound for the m^{th} energy bin. An initial lower energy bound of 0 MeV is implied. The user must then specify energy bins and corresponding weights for all energies from 0 MeV to the maximum energy of the problem

as specified on the PHYS card (default is 100 MeV for photons). By assigning higher weights to particular energy bins, the user can preferentially sample energy regions of interest. In Fig. 2, energy biasing has been used to set the sampling frequency of the energy region around the 185.7 keV peak to 100 times that of all other energy regions. The result is a decrease in relative error for that energy region while surrounding regions exhibit higher relative errors due to decreased sampling frequency. Furthermore, the use of energy biasing does not significantly alter the integral gamma emissions for either case.

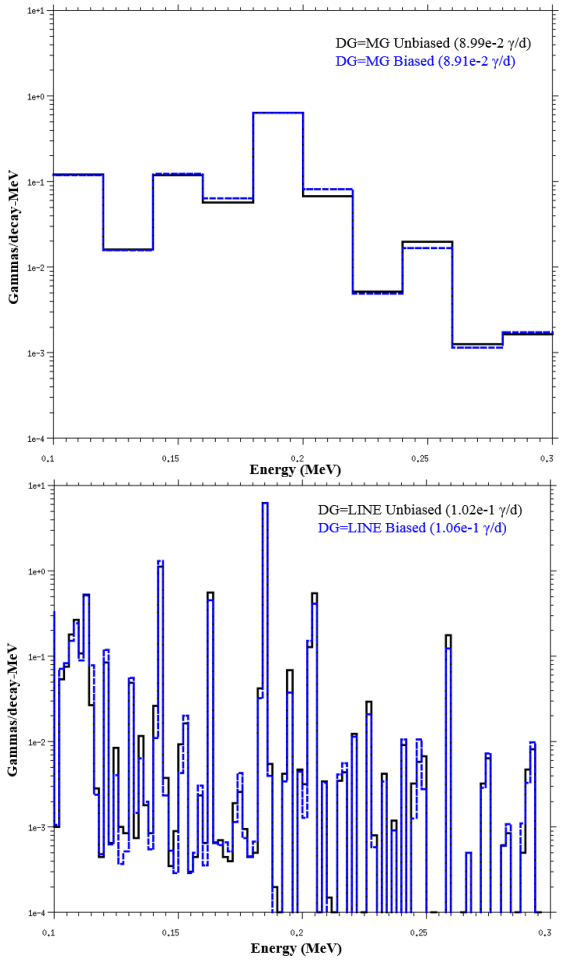

Fig. 2 – Effects of biasing the 185.7 keV peak with multi-bin gamma sampling (top) and line-emission sampling (bottom). Integral values are provided in parenthesis.

GAMMA-RAY SPECTROSCOPY EXAMPLE

In order to demonstrate the effectiveness of delayed-gamma energy biasing with line-emission sampling in MCNP6, a study was created in which energy biasing is used to improve convergence time in uranium enrichment calculations based on characteristic gamma-ray signatures.

The quantity of a target isotope in a given material can be determined by measuring the number of characteristic gamma emissions using the following expression:

$$N_i = \frac{C_\gamma \times \varepsilon_\gamma}{\lambda_i \times I_\gamma} \quad [1]$$

where C_γ is the total number of counts for a characteristic gamma energy (γ), ε_γ is the detector efficiency at that energy, λ_i is the decay constant of the target isotope, I_γ is the branching ratio for emission of gamma energy γ, and N_i is the total number of atoms of the isotope.

Following the alpha decay of U-238 (Th-231) and U-238 (Pa-234m), gamma rays are emitted at energies of 185.7 keV and 1001 keV, respectively [4]. By counting the number of gammas released at these two energies, the number of the uranium isotopes U-235 and U-238 can be determined using Equation 1 and the enrichment calculated by:

$$En_{235} = \frac{N_{235}}{N_{238}+N_{235}} \quad [2]$$

where N_{235} and N_{238} are the measured number U-235 and U-238 atoms using the counts associated with the 185.7 and 1001 keV gamma rays, respectively.

MCNP6 simulations were performed in which the U-235 enrichment of a sample was measured using the technique described above. For each sample simulation, an MCNP input deck was created with a 0.01 cm radius sphere (~22 μg) composed of a different enrichment. The uranium enrichment information used in this study was based on the National Bureau of Standards Standard Reference Material (SRM) 969 [5] which provides U-234, U-235, U-236, and U-238 isotopic concentrations for five enrichments ranging from 0.31% to 4.46% and from the New Brunswick Laboratory CRM 146 Uranium Isotopic Standard for Gamma Spectroscopy Measurements [6] which provides isotopic information for enrichments of 20.11%, 52.48% and 93.17%. The mass percent of each uranium isotope for the various enrichment standards used are provided in Table 1.

Table 1 – Uranium enrichments in mass percent

U^{235}/U	U^{234}	U^{235}	U^{236}	U^{238}
0.31	0.002	0.3166	0.0146	99.6668
0.71	0.0052	0.7119	0.00002	99.2828
1.94	0.0171	1.9420	0.0003	98.0406
2.95	0.0279	2.9492	0.0033	97.0196
4.46	0.0359	4.4623	0.0068	95.4950
20.11	0.14861	20.107	0.1973	79.547
52.48	0.3718	52.488	0.26495	46.876
93.17	0.9800	93.1703	0.2937	5.5559

Gamma emissions were counted with surface current (F1) tallies located on the outer radius of the uranium sphere. Three F1 tallies were used in total. One broad energy tally over a range of 0 to 3 MeV, and two narrow energy tallies around the lines of interest, with ranges from 0.185 to 0.186 and 1.0005 and 1.0015 respectively.

Three separate analysis were performed with line-emission delayed-gamma sampling for each enrichment case. In the first analysis, a control group was established by running each case without biasing. In the second analysis, the energy regions of interest were each given an equal weight of 1 while the weight in all other regions was lowered to 0.01. In the final analysis the relative emission frequency of each line based on activity was taken into account and weights were adjust for each energy region of interest accordingly. A comparison of the computational performance was performed for all three methods using the figure-of-merit (FOM) metric provided in the tally fluctuation chart (TFC), which is given by:

$$FOM \equiv \frac{1}{T\,R^2} \qquad [3]$$

where T is the total run time and R is the relative error of the tally. By default, the FOM will be calculated for the total (integral) bin for each tally. Therefore to find the FOM for the energy regions of interest the 7th entry on the tally fluctuation (TF*n*) card was used to specify the energy bin for which the TFC statistical information is calculated. When comparing FOMs to determine computational efficiency, it is important to note that, because T is in the denominator, the FOM is system dependent and therefore each simulation must be performed with the same computational system.

The emission probabilities of the 185.7 and 1001.3 keV particles were taken from the MCNP data file, cindergl.dat, and were 57.2% and 0.84%, respectively [7], while the half-lives for U-235 and U-238 were 703.8 million and 4.468 billion years, respectively. Using these values and the measured tallies of each gamma particle, the enrichment estimation was calculated using Equations 1 and 2. Each simulation was carried out until a relative error of ~5% or below was obtained in the enrichment calculation for each case.

RESULTS

Tally bin data for the natural uranium and 52% enriched uranium is shown in Fig. 3, highlighting the two peaks utilized for the enrichment calculation. Note the difference in magnitude of the 1001 keV peak between natural and 52% enriched uranium, indicating a decreased sampling frequency as U-235 enrichment is increased.

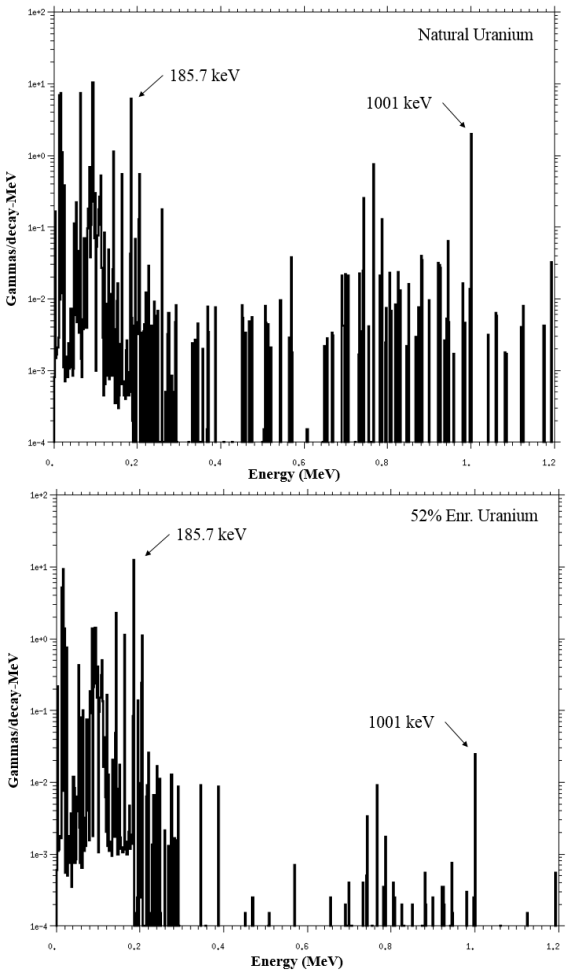

Fig. 3 – Delayed gamma spectrum of natural (top) and 52% enriched uranium (bottom).

Computational performance results using the FOMs for each case are provided in Fig. 4 for the 185.7 keV and 1001 keV gamma lines. In the case of the 185.7 keV line, FOM values remain fairly constant are nearly identical for the unbiased and equally-biased cases. This is because in the unbiased case the emission frequency is simply the true probability, 57.2%, and in the equally weighted case the emission frequency is roughly the same at ~50%. A decrease in the FOM value is seen for the adjusted-biasing case as the enrichments increase. This is a result of decreased sampling frequency of the 185.7 keV region due to the increased biasing applied to the 1001 keV region for higher enrichment cases. FOM values for the 1001 keV energy region show a downward trend with increased enrichment due to smaller quantities of U-238. Equal biasing improves the FOM for each enrichment bcause the sampling frequency of the 1001 keV line is increase from the true probability of 0.84% to ~50%. The adjusted biasing shows an improvement over equal biasing at enrichments of 4.46% above due to the sampling frequency being increased to greater than 50% through biasing.

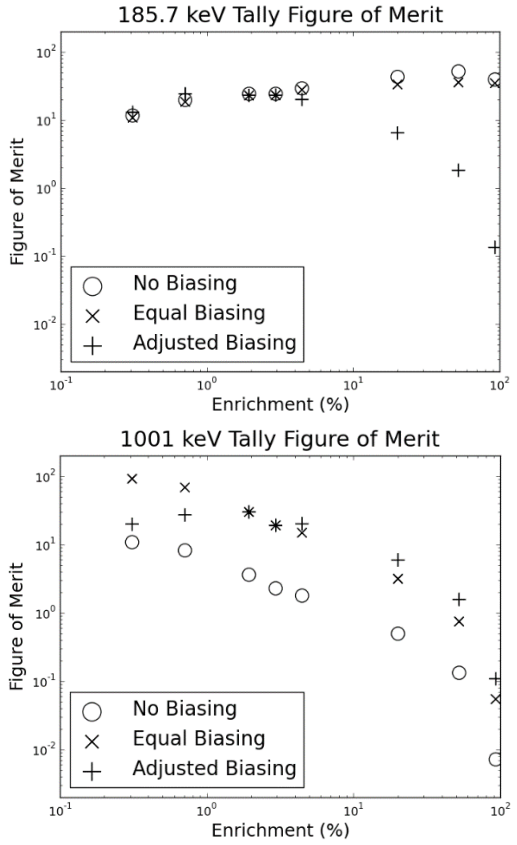

Fig. 4 – Figure of merits for 185.7 keV (top) and 1001 keV (bottom) tallies using line-emission sampling

Table 2 – Estimated enrichment calculation from the MCNP6 line-emission simulation. REs shown in parenthesis.

ENRICHMENT	NO BIASING	BIASING
0.31	0.32 (0.02)	0.32 (0.01)
0.71	0.71 (0.02)	0.72 (0.01)
1.94	1.96 (0.03)	1.96 (0.01)
2.95	3.04 (0.03)	3.00 (0.01)
4.46	4.60 (0.03)	4.50 (0.01)
20.11	20.29 (0.04)	20.81 (0.03)
52.48	53.08 (0.05)	53.76 (0.05)
93.17	93.10 (0.06)	92.94 (0.06)

Enrichment calculations from the MCNP simulation are provided in Table 2 and show good agreement. Similar results were found between the unbiased, equally-biased, and adjusted-biasing case showing that the introduction of biasing does not significantly influence results.

CONCLUSION

The delayed-gamma feature in MCNP6.2.0 with line-emission sampling provided a reasonable means for simulating the measurement of uranium enrichment using gamma-ray spectroscopy. Of practical importance, the application of delayed-gamma energy biasing was shown to improve the computational performance, specifically in cases where there a target delayed-gamma emission has very low emission probability. This is the case for the high enriched uranium examples, where the 1001 keV delayed gamma from U-238 is emitted orders of magnitude less frequently than the 185.7 keV particle from U-235, in contrast to their comparable emission probabilities in natural uranium.

ACKNOWLEDGEMENTS

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