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Author(s): Russell D. Mosteller

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Impact of MCNP Unresolved Resonance Probability-Table Treatment on ^{233}U Benchmarks

Russell D. Mosteller
Advanced Nuclear Technology Group (NIS-6)
Nonproliferation and International Security Division
Los Alamos National Laboratory

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Impact of MCNP Unresolved Resonance Probability-Table Treatment on ^{233}U Benchmarks

Russell D. Mosteller

Los Alamos National Laboratory

Previous versions of the MCNP Monte Carlo code,¹ up through and including MCNP4B, have not accurately modeled neutron self-shielding effects in the unresolved resonance energy region. Recently, a probability-table treatment² has been incorporated into an intermediate version called MCNP4XS, and compatible continuous-energy cross-section libraries have been developed for 27 different isotopes.³ Preliminary results for a variety of uranium and plutonium benchmarks have been presented previously,⁴ and this paper extends those results to include several ^{233}U benchmarks.

The probability-table method^{5,6} relies on the statistical nature of neutron resonances in the unresolved region. Average unresolved resonance parameters from nuclear-data evaluations may be utilized by a processing code (in this case, NJOY⁷) to generate ladders of representative resonances. Cross sections from these ladders then are used to form cross-section probability distribution functions, from which NJOY prepares a table of cross sections (total, elastic, fission, radiative capture, and heating) as a function of probability. Such tables are a function of incident neutron energy. When transporting neutrons in the unresolved energy range of a particular nuclide, MCNP4XS samples the total and reaction cross sections rather than simply using single average values as the code has done in the past. By virtue of randomly sampling large, intermediate, and small cross sections from the probability tables, MCNP4XS models the effects of neutron self-shielding in the unresolved resonance energy region.

The previous results were obtained using a preliminary set of cross-section libraries that contained probability tables only for ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu , and ^{242}Pu . In contrast, the final libraries contain probability tables for 27 isotopes, including ^{233}U . All the previous benchmarks have been re-run with the final libraries, and, although there are small differences between many of the new and old eigenvalues, the conclusions that were drawn from the preliminary results all remain valid. The most important of those conclusions are that (1) the probability-table method does not significantly affect the reactivity results for highly enriched uranium (i.e., ^{235}U) systems, but (2) MCNP calculations for systems with large amounts of ^{238}U and intermediate spectra can produce significantly nonconservative results unless the probability-table method is employed.

The objective of the current study is to assess the reactivity impact of the probability-table treatment on ^{233}U systems. The benchmarks that were chosen are summarized in Table 1. With three exceptions, they employ specifications⁸ provided by the Working Group for the International Criticality Safety Benchmark Evaluation Program (ICSBEP). Unfortunately, neither the ICSBEP benchmarks nor those⁹ from the Cross Section Evaluation Working Group include any ^{233}U systems with intermediate spectra, and inclusion of cases with intermediate effects is necessary for this study because the unresolved resonance region for ^{233}U extends from 60 eV to 10 keV. Consequently, three fictitious cases — ^{233}U ZEBRA 8H, ^{233}U HUG #1, and ^{233}U HUG #2 — were constructed from the ICSBEP $^{235}\text{U}/^{238}\text{U}$ k_{∞} benchmarks for ZEBRA 8H (MIX-MET-FAST-008) and HISS/HUG (HEU-COMP-INTER-004). ZEBRA 8H, while predominantly a fast system, contains a significant intermediate tail, while the HUG cases have spectra that overlap the entire unresolved resonance range of the ^{233}U . The ^{233}U density in case #2 is only half that in case #1, and consequently it has a somewhat softer spectrum.

The MCNP4XS calculations each used 1 million active histories, and employed ENDF/B-VI cross-section libraries exclusively. In contrast to the previously distributed ENDF60 library,¹⁰ which is consistent with release 2 of ENDF/B-VI, the libraries with probability tables all are consistent with Release 4. With the exception of the three fictitious cases, the calculations always employed cross sections with probability tables for the isotopes that have them, and the cross sections for all other isotopes were taken from ENDF60. However, because they are strictly computational benchmarks, in the calculations for ²³³U ZEBRA 8H and the ²³³U HUG cases probability tables were employed only for ²³³U to isolate the effects on it.

The results from these calculations, along with their associated standard deviations, are presented in Table 2. Not surprisingly, results for the fast and thermal benchmarks are not significantly affected. Specifically, the spectra for the metal spheres and for ²³³U ZEBRA 8H are too hard to produce large reactivity changes, while the spectrum for the nitrate solution is too thermal. The probability-table method produces a significant change in reactivity for ²³³U HUG #1 but, at most, a marginal change for ²³³U HUG #2. This result demonstrates that the probability-table method can have a small but significant reactivity impact for ²³³U systems with spectra that substantially overlap the unresolved resonance range for ²³³U. However, the magnitude of that impact is quite sensitive to the details of the spectrum even within that range.

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Table 1. Summary of ^{233}U Benchmarks

Benchmark Name	ICSBEP Identifier	Principal Core Material(s)	Principal Reflector Material(s)	Shape
Jezebel-23	U233-MET-FAST-001	Uranium (98.13 wt.% ^{233}U)	None	Sphere
FLATTOP-23	U233-MET-FAST-006	Uranium (98.13 wt.% ^{233}U)	Normal U	Sphere
^{233}U Reflected by Tungsten	U233-MET-FAST-004, Case 2	Uranium (98.2 wt.% ^{233}U)	Tungsten	Sphere
^{233}U Reflected by Beryllium	U233-MET-FAST-005, Case 2	Uranium (98.2 wt.% ^{233}U)	Beryllium	Sphere
^{233}U ZEBRA 8H	None	Uranium (20.5 wt.% ^{233}U), Normal U (6 wt.% ^{233}U Average)	Steel	Infinite Lattice of Parallelepipeds
^{233}U HUG #1	None	Uranium (45.9 wt.% ^{233}U), Graphite, Boron	—	Infinite, Homogeneous
^{233}U HUG #2	None	Uranium (45.9 wt.% ^{233}U), Graphite, Boron	—	Infinite, Homogeneous
ORNL-9	U233-SOL-THERM-001, Case 5	Uranyl Nitrate (97.7 wt.% ^{233}U), Water	None	Cylinder

Table 2. Reactivity Impact of Probability-Table Treatment for ^{233}U Systems

Benchmark Name	k_{eff} or k_{∞}			Δk_{PT}
	Benchmark	with Probability Tables	without Probability Tables	
Jezebel-23	1.0000 ± 0.0010	0.9930 ± 0.0006	0.9928 ± 0.0005	0.0002 ± 0.0008
FLATTOP-23	1.0000 ± 0.0014	1.0007 ± 0.0007	1.0000 ± 0.0006	0.0007 ± 0.0009
^{233}U Reflected by Tungsten	1.0000 ± 0.0007	1.0049 ± 0.0006	1.0050 ± 0.0007	-0.0001 ± 0.0009
^{233}U Reflected by Beryllium	1.0000 ± 0.0030	0.9976 ± 0.0007	0.9982 ± 0.0006	-0.0006 ± 0.0009
^{233}U ZEBRA 8H	—	0.9931 ± 0.0004	0.9928 ± 0.0004	0.0003 ± 0.0006
^{233}U HUG #1	—	1.0350 ± 0.0005	1.0379 ± 0.0006	-0.0029 ± 0.0008
^{233}U HUG #2	—	1.0365 ± 0.0006	1.0374 ± 0.0006	-0.0009 ± 0.0008
ORNL-9	1.0004 ± 0.0033	0.9971 ± 0.0006	0.9965 ± 0.0006	0.0006 ± 0.0008