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on

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IMPACT OF MCNP UNRESOLVED RESONANCE PROBABILITY-TABLE TREATMENT ON URANIUM AND PLUTONIUM BENCHMARKS

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Abstract

A probability-table treatment recently has been incorporated into an intermediate version of the MCNP Monte Carlo code named MCNP4XS. This paper presents MCNP4XS results for a variety of uranium and plutonium criticality benchmarks, calculated with and without the probability-table treatment. It is shown that the probability-table treatment can produce small but significant reactivity changes for plutonium and ^{233}U systems with intermediate spectra. More importantly, it can produce substantial reactivity increases for systems with large amounts of ^{238}U and intermediate spectra.

Versions of the MCNP Monte Carlo code[1] up through and including 4B have not accurately modeled neutron self-shielding effects in the unresolved resonance energy region. Recently, a probability-table treatment has been incorporated into a version intermediate between 4B and 4C named MCNP4XS.[2] This paper presents MCNP4XS results for a variety of uranium and plutonium criticality benchmarks, calculated with and without the probability-table treatment.

The probability-table method[3,4] 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, NJOY[5]) 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 cross sections for isotopes with probability-table data are consistent with ENDF/B-VI release 4 (Ref. 6), and the unresolved resonance ranges for the uranium and plutonium isotopes that are relevant to this study are given in Table 1. Cross sections for all other isotopes in the benchmarks were from the distributed ENDF60 library,[7] which is based on ENDF/B-VI release 2 and does not include probability tables. However, ^{14}N and ^{17}Al are the only such isotopes without probability tables whose evaluations were revised between ENDF/B-VI releases 2 and 4. Furthermore, the changes to ^{14}N all were above 13 MeV and therefore are not relevant to this study. Aluminum appears only as a container in a few of the benchmarks, and the impact of changes to its cross sections probably is negligible. Consequently, the results obtained in this study are generally representative of ENDF/B-VI release 4.

Several uranium and plutonium benchmarks were selected to assess the reactivity impact of the probability-table method. The benchmarks, which are summarized in Tables 2, 3, 4, and 5, include highly enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), plutonium, mixed uranium-plutonium, and ^{233}U cores that produce a range of neutron spectra. Most of these benchmarks are based on specifications provided by the Cross Section Evaluation Working Group[8] (CSEWG) or the Working Group for the International Criticality Safety Benchmark Evaluation Program[9] (ICSBEP). Table 6 briefly summarizes some fictional configurations that were constructed to provide additional testing of the probability-table enhancements for plutonium and for ^{233}U systems.

Each MCNP4XS calculation employed 250 generations of 5,000 neutrons each. The first 50 generations were excluded from the statistics, thereby producing 1 million active histories for each calculation.

The results from the calculations for the HEU benchmarks are shown in Table 7, along with their associated standard deviations (1-σ). Even though the fluxes for ZEUS, HISS/HUG, and the uranium hydride (UH_3) benchmark are quite high within the unresolved resonance range for ^{235}U, none of the reactivity differences are statistically significant. Consequently, it can be concluded that the probability-table treatment does not significantly affect the results for HEU benchmarks.

The results for the IEU and LEU benchmarks are given in Table 8. The probability-table treatment produces significant changes in reactivity for all of these benchmarks except the graphite-reflected IEU sphere, which has a predominantly fast spectrum, and SHEBA-II and ORNL-4, which have predominantly thermal spectra. The magnitude of the reactivity change in the remaining benchmarks depends primarily upon the amount of ^{238}U present, its location, and the amount of overlap between the spectrum and the unresolved resonance range for ^{238}U.

None of the results for the plutonium benchmarks presented in Table 9 show a statistically significant difference for the probability table treatment. This behavior is expected for both Jezebel cases, which have fast spectra, and for PNL-2, which has a thermal spectrum. However, both VERA-11A and HISS/HPG have intermediate spectra. The impact of the probability-table treatment for plutonium systems will be discussed further below.

Results for the mixed uranium-plutonium benchmarks are shown in Table 10. All of these benchmarks have intermediate spectra, and the reactivity changes for most of them are substantial. The large reactivity differences, like those for the IEU cases, are almost entirely to ^{238}U.

Two further observations can be made with regard to the results for the mixed uranium-plutonium benchmarks and the IEU benchmarks with intermediate spectra. First, the reactivity changes all are in the positive direction, which demonstrates that results for cases with intermediate spectra and large amounts of ^{238}U will be *nonconservative* unless the probability-table treatment is employed. Second, the results without the probability-table treatment are in markedly better agreement with the benchmark values than are those with it. This pattern implies that ENDF/B-VI underestimates capture in ^{238}U in the unresolved resonance range. This conclusion is somewhat surprising, because two recent studies[10,11] indicate that ENDF/B-VI may overestimate the resonance integral for ^{238}U. Taken together, these studies strongly suggest that the ENDF/B-VI specifications for ^{238}U should be reviewed throughout the resolved and unresolved resonance ranges.

The results for the ^{233}U systems are presented in Table 11. Unfortunately, none of the CSEWG or ICSBEP benchmarks for ^{233}U include has an intermediate spectrum. Specifically, the spectra for the metal spheres are too hard to produce large reactivity changes, while the spectrum for the nitrate solution is too thermal.

Because the plutonium and ^{233}U benchmarks did not produce conclusive evidence of the reactivity impact (or lack thereof), a series of fictitious systems was generated. These systems were based on the ZEBRA 8H, HISS/HUG, HISS/HPG, and VERA-11A benchmarks but were altered to produce spectra that better matched the unresolved resonance ranges for those isotopes. Because these cases are strictly computational benchmarks, probability tables were employed only for ^{233}U and the plutonium isotopes to isolate the effects upon them.

Most of these fictitious systems continued to show no significant differences between the cases with probability tables and those without. However, as Table 12 demonstrates, the modified VERA-11A case and the ^{233}U HUG cases produce significant differences in reactivity. These results demonstrate that the probability-table method can have a small but significant reactivity impact for plutonium and ^{233}U systems with spectra that substantially overlap their unresolved resonance ranges. However, the magnitude of that impact is quite sensitive to the details of the spectrum even within that range.

The following conclusions can be drawn from the results of this study:

(1) Not surprisingly, the only benchmarks that are substantially affected are those that have a significant fraction of their interactions within the unresolved resonance region of the principal uranium and plutonium isotopes that are present;

(2) the reactivity impact of the improvement is essentially negligible for HEU systems;

(3) the probability-table method can produce small but significant changes in reactivity for plutonium and ^{233}U systems, but the magnitude of that impact is quite sensitive to the spectral details;

(4) the probability-table method can produce substantial increases in reactivity for systems that include large amounts of ^{238}U and have high fluxes within the unresolved resonance region, which indicates that calculations for such systems will produce significantly *nonconservative* results unless the probability-table treatment is employed; and

(5) these results, in conjunction with those obtained in previous studies, strongly suggest that the ENDF/B-VI specifications for ^{238}U need to be reviewed.

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Table 1. Unresolved Resonance Regions for Uranium and Plutonium Isotopes

Isotope	Lower Limit (keV)	Upper Limit (keV)
^{234}U	1.5	100
^{235}U	2.25	25
^{236}U	1.5	100
^{238}U	10	149.03
^{239}Pu	2.5	30
^{240}Pu	5.7	40
^{241}Pu	0.3	40.2
^{242}Pu	0.986	10

Table 2. Summary of Uranium Benchmarks

Benchmark Name	Identifier	Principal Core Material(s)	Principal Reflector Material(s)	Shape
GODIVA	CSEWG FRB 5	HEU (93 wt.%)	None	Sphere
ZPR-9-34	ICSBEP HEU-MET-FAST-035	HEU (93 wt.%), Steel	Steel	Cylinder
VERA-1B	CSEWG FRB 6	HEU (93 wt.%), Graphite	Normal U, Steel	Sphere
ZEUS*	—	HEU (93 wt.%), Graphite	Copper	Cylinder
ORNL-4	ICSBEP HEU-SOL-THERM-013	HEU (93 wt.%) Nitrate Solution	None	Sphere
UH_3 Number 4*	ICSBEP HEU-COMP-INTER-003	HEU (93 wt.%) Hydride	Depleted U, Iron	Cylinder
HISS/HUG	ICSBEP HEU-COMP-INTER-004	HEU (92 wt.%), Graphite, Boron	—	Infinite
ZPR-III-2	CSEWG FRB 7	IEU (46 wt.%), Steel	Normal U, Steel	Cylinder
ZPR-III-6F	CSEWG FRB 7	IEU (46 wt.%), Steel	Normal U, Steel	Cylinder
GRIEUS**	ICSBEP IEU-MET-FAST-004	IEU (36 wt.%)	Graphite	Sphere
ZPR-III-12	CSEWG FRB 9	IEU (21 wt.%), Graphite	Depleted U, Steel	Cylinder
ZEBRA-2	CSEWG FRB 10	IEW (13.7 wt.%), Graphite	Normal U	Cylinder
ZPR-III-11	CSEWG FRB 8	IEU (12 wt.%), Steel	Normal U, Steel	Cylinder
BIG TEN	CSEWG FRB 20	IEU (10 wt.%)	Depleted U	Sphere
ZEBRA-8H	ICSBEP MIX-MET-FAST-008	IEU (37.5 wt.%), Normal U (6 wt.% Average)	Steel	Infinite Lattice of Parallelepipeds
SHEBA-II	ICSBEP LEU-SOL-THERM-001	LEU (5 wt.%) Uranyl Fluoride, Water	None	Cylinder

* Preliminary specifications

** Acronym for Graphite-Reflected Intermediate-Enriched Uranium Sphere

Table 3. Summary of Plutonium Benchmarks

Benchmark Name	Identifier	Principal Core Material(s)	Principal Reflector Material(s)	Shape
JEZEBEL	CSEWG FRB 1	Pu (4.5 at.% ^{24}0Pu)	None	Sphere
JEZEBEL-240	CSEWG FRB 21	Pu (20.1 at.% ^{240}Pu)	None	Sphere
VERA-11A	CSEWG FRB 2	Pu (4.9 at.% ^{240}Pu)	Normal U, Steel	Cylinder
HISS/HPG	ICSBEP PU-COMP-INTER-001	Pu (5.3 at.% ^{240}Pu), Graphite, Boron	——	Infinite
PNL-2	ICSBEP PU-SOL-THERM-021	Pu (2.5 at.% ^{240}Pu) Nitrate, Water	None	Sphere

Table 4. Summary of Mixed Uranium-Plutonium Benchmarks

Benchmark Name	Identifier	^{240}Pu (at.%)	Uranium	Principal Reflector Material(s)	Shape
ZEBRA-8A/2	ICSBEP MIX-MET-FAST-008	4.9	Normal U	——	Infinite Lattice of Parallelepipeds
ZEBRA-8B	ICSBEP MIX-MET-FAST-008	4.9	Normal U	——	Infinite Lattice of Parallelepipeds
ZEBRA-8C/2	ICSBEP MIX-MET-FAST-008	4.9	Normal U	——	Infinite Lattice of Parallelepipeds
ZEBRA-8D	ICSBEP MIX-MET-FAST-008	4.9	Normal U	——	Infinite Lattice of Parallelepipeds
ZEBRA-8E	ICSBEP MIX-MET-FAST-008	4.9	Normal U	——	Infinite Lattice of Parallelepipeds
ZEBRA-8F/2	ICSBEP MIX-MET-FAST-008	9.9*	Normal U**	——	Infinite Lattice of Parallelepipeds
ZPR-III-48	CSEWG FRB 3	6.0	Depleted U	Depleted U, Steel	Cylinder

* MOX (25 wt.% PuO_2)   ** UO_2

Table 5. 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
ORNL-9	U233-SOL-THERM-001, Case 5	Uranyl Nitrate (97.7 wt.% ^{233}U), Water	None	Cylinder

Table 6. Summary of Fictitious Plutonium and ^{233}U Systems

Name	Principal Core Material(s)	Principal Reflector Material(s)	Shape
VERA-11A Modified	Pu (4.9 at.% ^{240}Pu), Graphite	Normal U, Steel	Cylinder with Infinite Reflector
^{233}U HUG #1	Uranium (45.9 wt.% ^{233}U), Graphite, Boron	—	Infinite, Homogeneous
^{233}U HUG #2	Uranium (45.9 wt.% ^{233}U), Graphite, Boron	—	Infinite, Homogeneous

Table 7. Results for HEU Benchmarks

Benchmark Name	k_{eff} or k_∞			Δk_{PT}
	Benchmark	with Probability Tables	without Probability Tables	
GODIVA	1.0000 ± 0.0030	0.9959 ± 0.0006	0.9961 ± 0.0006	-0.0002 ± 0.0008
ZPR-9-34	0.9966 ± 0.0028	1.0090 ± 0.0007	1.0095 ± 0.0006	-0.0005 ± 0.0009
VERA-1B	1.0000 ± 0.0028	1.0011 ± 0.0006	1.0014 ± 0.0007	-0.0003 ± 0.0009
ZEUS	—	1.0058 ± 0.0009	1.0060 ± 0.0007	-0.0002 ± 0.0011
UH_3 Number 4	1.0000 ± 0.0065	1.0008 ± 0.0008	1.0012 ± 0.0008	-0.0004 ± 0.0011
HISS/HUG	1.0000 ± 0.0040	1.0147 ± 0.0005	1.0140 ± 0.0005	0.0007 ± 0.0007
ORNL-4	1.0003 ± 0.0036	0.9934 ± 0.0006	0.9942 ± 0.0006	-0.0008 ± 0.0008

Table 8. Results for IEU and LEU Benchmarks

Benchmark Name	k_{eff} or k_∞			Δk_{PT}
	Benchmark	with Probability Tables	without Probability Tables	
ZPR-III-2	1.0000 ± 0.0015	1.0041 ± 0.0006	1.0017 ± 0.0006	0.0024 ± 0.0008
ZPR-III-6F	0.9966 ± 0.0015	1.0054 ± 0.0006	1.0029 ± 0.0007	0.0025 ± 0.0009
GRIEUS	1.0000 ± 0.0030	1.0047 ± 0.0006	1.0043 ± 0.0006	0.0004 ± 0.0008
ZPR-III-12	1.0	1.0075 ± 0.0006	1.0031 ± 0.0006	0.0044 ± 0.0008
ZEBRA-2	1.0000 ± 0.0020	1.0041 ± 0.0005	0.9989 ± 0.0005	0.0052 ± 0.0007
ZPR-III-11	1.0000 ± 0.0025	1.0166 ± 0.0005	1.0142 ± 0.0004	0.0024 ± 0.0006
BIG TEN (2D)	0.9960 ± 0.0030	1.0132 ± 0.0005	1.0084 ± 0.0005	0.0048 ± 0.0007
ZEBRA-8H	1.0300 ± 0.0025	1.0418 ± 0.0004	1.0303 ± 0.0004	0.0115 ± 0.0006
SHEBA-II	0.9991 ± 0.0029	1.0102 ± 0.0008	1.0093 ± 0.0008	0.0009 ± 0.0011

Table 9. Results for Plutonium Benchmarks

Benchmark Name	k_{eff} or k_∞			Δk_{PT}
	Benchmark	with Probability Tables	without Probability Tables	
JEZEBEL	1.0000 ± 0.0030	0.9983 ± 0.0006	0.9981 ± 0.0006	0.0002 ± 0.0008
JEZEBEL-240	1.0000 ± 0.0030	0.9992 ± 0.0006	0.9991 ± 0.0006	0.0001 ± 0.0008
VERA-11A	1.0000 ± 0.0030	0.9910 ± 0.0007	0.9915 ± 0.0006	-0.0005 ± 0.0009
HISS/HPG	1.0000 ± 0.0100	1.0117 ± 0.0005	1.0115 ± 0.0005	0.0002 ± 0.0007
PNL-2	1.0000 ± 0.0065	1.0017 ± 0.0011	1.0005 ± 0.0010	0.0012 ± 0.0015

Table 10. Results for Mixed Uranium-Plutonium Benchmarks

Benchmark Name	k_{eff} or k_∞			Δk_{PT}
	Benchmark	with Probability Tables	without Probability Tables	
ZEBRA-8A/2	0.9920 ± 0.0063	1.0041 ± 0.0005	0.9924 ± 0.0005	0.0117 ± 0.0007
ZEBRA-8B	1.0010 ± 0.0023	1.0167 ± 0.0004	1.0055 ± 0.0005	0.0112 ± 0.0006
ZEBRA-8C/2	0.9860 ± 0.0044	0.9961 ± 0.0004	0.9870 ± 0.0005	0.0091 ± 0.0006
ZEBRA-8D	0.9730 ± 0.0045	0.9892 ± 0.0005	0.9767 ± 0.0005	0.0125 ± 0.0007
ZEBRA-8E	1.0060 ± 0.0069	1.0056 ± 0.0004	0.9935 ± 0.0004	0.0121 ± 0.0006
ZEBRA-8F/2	0.9710 ± 0.0042	0.9819 ± 0.0004	0.9775 ± 0.0004	0.0044 ± 0.0006
ZPR-III-48	0.9817 ± 0.0010	0.9932 ± 0.0006	0.9887 ± 0.0006	0.0045 ± 0.0008

Table 11. 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
ORNL-9	1.0004 ± 0.0033	0.9971 ± 0.0006	0.9965 ± 0.0006	0.0006 ± 0.0008

Table 12. Reactivity Impact of Probability-Table Treatment for Fictitious Plutonium and ^{233}U Systems

Name	k_{eff} or k_∞		Δk_{PT}
	with Probability Tables	without Probability Tables	
VERA-11A Modified	1.0186 ± 0.0006	1.0199 ± 0.0007	-0.0013 ± 0.0009
^{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