

LA-UR- 98-2873

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Title: ENDF/B-V and ENDF/B-VI Results for UO-2
Lattice Benchmark Problems Using MCNP

CONF-981003--

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Submitted to: International Conference on the Physics of
Nuclear Science and Technology
Islandia, Long Island, NY
October 5-8, 1998

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Form 836 (10/96)

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ENDF/B-V AND ENDF/B-VI RESULTS FOR UO₂ LATTICE BENCHMARK PROBLEMS USING MCNP

by

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(Expanded Version of LA-UR-98-0023)

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ABSTRACT

Calculations for the ANS UO₂ lattice benchmark have been performed with the MCNP Monte Carlo code and its ENDF/B-V and ENDF/B-VI continuous-energy libraries. The ENDF/B-V library produces significantly better agreement with the benchmark value for k_{eff} than do the ENDF/B-VI libraries. However, the pin power distributions are essentially the same irrespective of the library.

I. INTRODUCTION

Calculations for the ANS UO₂ lattice benchmark¹ have been performed with the MCNP Monte Carlo code² and its ENDF/B-V and ENDF/B-VI continuous-energy libraries. Similar calculations were performed previously³ for the experiments upon which these benchmarks are based, using continuous-energy libraries derived from ENDF/B-V and from Release 2 of ENDF/B-VI (ENDF/B-VI.2). This study extends those calculations to the infinite-lattice configurations given in the benchmark specifications and also includes results from Release 3 of ENDF/B-VI (ENDF/B-VI.3) for both the core and infinite-lattice configurations.

For this set of benchmarks, the only significant difference between the ENDF/B-VI.2 and ENDF/B-VI.3 libraries is the cross-section behavior of ²³⁵U. ENDF/B-VI.3 contains revised cross sections for ²³⁵U below 900 eV,⁴ although those changes principally affect the range below 110 eV.^{5,6} In particular, relative to ENDF/B-VI.2, ENDF/B-VI.3 increases the epithermal capture-to-fission ratio for ²³⁵U and slightly increases its thermal fission cross section.

Each MCNP case discussed herein was run with 4,000 particles per generation and 1,050 generations. The first 50 generations were excluded from the statistics, thereby

producing 4,000,000 active histories for each case. The core cases were run with an axial length of 163.324 cm, which corresponds to a geometric axial buckling of 0.00037 cm⁻². The infinite-lattice cases were run with reflective boundary conditions on all surfaces.

II. RESULTS FOR CORE CONFIGURATIONS

The values for k_{eff} for the core problems are reported in Table 1, along with the resulting differences from the benchmark value (1.0007 ± 0.0006). The pin power distributions in the central assembly of configurations B and C are shown in Figures 1 and 2, respectively.

ENDF/B-V appears to underpredict k_{eff} slightly for these cases. However, it has been reported⁷ that deficiencies in the MCNP ENDF/B-V library for ²³⁸U produce a bias of approximately $-.003 \Delta k$ in the calculated value of k_{eff} for thermal lattices with low-enriched UO₂ fuel. If that bias is applied to these results, ENDF/B-V produces excellent agreement with the benchmark value for k_{eff} : all three values for k_{eff} are within 2 standard deviations of the benchmark value, and the difference between the benchmark and calculated means is 0.0012 Δk or less.

The ENDF/B-VI results for k_{eff} are not as good as those from ENDF/B-V. The calculated values of k_{eff} are approximately half a percent too low, with the ENDF/B-VI.3 value slightly but consistently lower than the ENDF/B-VI.2 value.

The pin power distributions from the three libraries all are in good agreement with the measured values, with an RMS difference of approximately 2% between the measured and calculated sample means. However, it is likely that the size of these differences would decrease somewhat if additional Monte Carlo histories were run to reduce the standard deviations for the calculations.

III. RESULTS FOR INFINITE-LATTICE CONFIGURATIONS

The values for k_{eff} and the various spectral indices from the infinite-lattice calculations are reported in Table 2, and the corresponding pin power distributions are shown in Figures 3 and 4. Not surprisingly, the results from the infinite-lattice cases produce patterns that are similar to those observed for the core cases. The ENDF/B-V library produces eigenvalues that are consistently higher than those for the ENDF/B-VI libraries, and the ENDF/B-VI.3 eigenvalue is slightly but consistently lower than the ENDF/B-VI.2 eigenvalue. The power distributions from all three libraries, however, continue to be very similar.

The suspicion that all three libraries produce essentially the same power distributions for these benchmarks is buttressed by the deviations between the power distributions summarized in Table 3. The standard deviations between sample means produced by the libraries are approximately the same as the standard deviations for individual pins. It appears highly likely that, given enough histories, the three libraries would produce virtually indistinguishable pin power distributions.

However, there are subtle changes to the reactivity differences that reflect cross-section differences between the libraries. In particular, the reactivity differences between the ENDF/B-V and ENDF/B-VI results decrease slightly relative to the core cases, which suggests that leakage from the core to the reflector is slightly higher for the ENDF/B-VI cases. Such behavior is consistent with differences in the ENDF/B-V and ENDF/B-VI cross sections for ^{16}O at high energies.

Differences in the spectral indices also reflect cross-section differences between the libraries and thereby help to explain the observed reactivity differences. The values for ρ_{25} (ratio of fast to thermal capture in ^{235}U) are consistent with the epithermal ^{235}U capture-to-fission ratio in the three libraries (i.e., ρ_{25} is lowest for ENDF/B-VI.2 and highest for ENDF/B-VI.3). The results from both ENDF/B-VI libraries for ρ_{28} (ratio of fast to thermal capture in ^{238}U) and for the conversion ratio are higher than those from ENDF/B-V, and such behavior indicates higher neutron capture rates in ^{238}U (the ENDF/B-VI.3 values are slightly but consistently lower than their ENDF/B-VI.2 counterparts, reflecting the increased competition between ^{235}U and ^{238}U in the epithermal region). All three libraries produce essentially the same values for δ_{28} (ratio of fission in ^{238}U to fission in ^{235}U) but the ENDF/B-VI values for δ_{25} (ratio of fast to thermal fission in ^{235}U) are lower than those from the ENDF/B-V calculations. This combination suggests that the reactivity differences between

ENDF/B-VI and ENDF/B-V are due, at least in part, to increased fast capture in ^{238}U and decreased fast fission in ^{235}U .

IV. CONCLUSIONS

Overall, the ENDF/B-V library produces significantly better agreement with the benchmark values for k_{eff} than do either of the ENDF/B-VI libraries. The pin power distributions, however, are essentially the same irrespective of the library. Finally, the spectral indices from the infinite-lattice cases are consistent with the known cross-section behavior in the three libraries and help to explain the observed reactivity differences.

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Table 1. MCNP Results for Core Configurations.

Core	K _{eff}			Δk		
	ENDF/B-V	ENDF/B-VI.2	ENDF/B-VI.3	ENDF/B-V	ENDF/B-VI.2	ENDF/B-VI.3
A	0.9981 ± 0.0003	0.9963 ± 0.0003	0.9956 ± 0.0003	-0.0026 ± 0.0007	-0.0044 ± 0.0007	-0.0051 ± 0.0007
B	0.9988 ± 0.0003	0.9964 ± 0.0003	0.9957 ± 0.0003	-0.0019 ± 0.0007	-0.0043 ± 0.0007	-0.0050 ± 0.0007
C	0.9965 ± 0.0003	0.9944 ± 0.0003	0.9940 ± 0.0003	-0.0042 ± 0.0007	-0.0063 ± 0.0007	-0.0067 ± 0.0007

Table 2. MCNP Results for Infinite-Lattice Configurations.

Configuration	Parameter	ENDF/B-V	ENDF/B-VI.2	ENDF/B-VI.3
A	k_e	1.0582 ± 0.0003	1.0562 ± 0.0003	1.0560 ± 0.0003
	δ_{25}	0.1324 ± 0.0001	0.1309 ± 0.0001	0.1297 ± 0.0001
	δ_{28}	0.0647 ± 0.0001	0.0649 ± 0.0001	0.0649 ± 0.0001
	ρ_{25}	0.3475 ± 0.0003	0.3374 ± 0.0003	0.3619 ± 0.0004
	ρ_{28}	2.2774 ± 0.0023	2.2980 ± 0.0024	2.2923 ± 0.0024
	CR*	0.4676 ± 0.0003	0.4726 ± 0.0003	0.4710 ± 0.0004
B	k_e	1.0486 ± 0.0003	1.0471 ± 0.0003	1.0466 ± 0.0003
	δ_{25}	0.1176 ± 0.0001	0.1163 ± 0.0001	0.1153 ± 0.0001
	δ_{28}	0.0600 ± 0.0001	0.0601 ± 0.0001	0.0601 ± 0.0001
	ρ_{25}	0.3089 ± 0.0003	0.2999 ± 0.0003	0.3211 ± 0.0003
	ρ_{28}	2.0282 ± 0.0021	2.0494 ± 0.0023	2.0448 ± 0.0023
	CR*	0.4380 ± 0.0003	0.4427 ± 0.0003	0.4414 ± 0.0003
C	k_e	0.9860 ± 0.0003	0.9850 ± 0.0003	0.9842 ± 0.0003
	δ_{25}	0.1307 ± 0.0001	0.1293 ± 0.0001	0.1282 ± 0.0001
	δ_{28}	0.0656 ± 0.0001	0.0656 ± 0.0001	0.0658 ± 0.0001
	ρ_{25}	0.3442 ± 0.0004	0.3339 ± 0.0004	0.3585 ± 0.0004
	ρ_{28}	2.2729 ± 0.0025	2.2874 ± 0.0025	2.2859 ± 0.0025
	CR*	0.4670 ± 0.0004	0.4710 ± 0.0004	0.4700 ± 0.0004
	PAF**	0.1393 ± 0.0002	0.1387 ± 0.0002	0.1389 ± 0.0002

* Conversion Ratio

** Pyrex Absorption Fraction

Table 3. RMS Differences between Libraries

Case	ENDF/B-V vs ENDF/B-VI.2	ENDF/B-V vs ENDF/B-VI.3	ENDF/B-VI.2 vs ENDF/B-VI.3
Core B	0.016	0.011	0.015
Core C	0.016	0.017	0.018
Infinite Lattice B	0.004	0.003	0.004
Infinite Lattice C	0.003	0.003	0.003

Figure 1. Pin Power Distribution in Central Assembly of Core B.

Figure 2. Pin Power Distribution in Central Assembly of Core C.

Water	1.051 \pm 0.004	0.998 \pm 0.003	0.977 \pm 0.003	0.970 \pm 0.003	0.979 \pm 0.003	0.953 \pm 0.003	0.946 \pm 0.003
Hole	1.060 \pm 0.004	0.998 \pm 0.003	0.975 \pm 0.003	0.971 \pm 0.003	0.979 \pm 0.003	0.961 \pm 0.003	0.948 \pm 0.003
	1.054 \pm 0.004	0.996 \pm 0.003	0.972 \pm 0.003	0.971 \pm 0.003	0.978 \pm 0.003	0.959 \pm 0.003	0.944 \pm 0.003
	1.020 \pm 0.003	1.051 \pm 0.002	1.003 \pm 0.002	0.999 \pm 0.002	1.040 \pm 0.002	0.980 \pm 0.002	0.945 \pm 0.002
	1.028 \pm 0.003	1.049 \pm 0.002	0.998 \pm 0.002	0.998 \pm 0.002	1.041 \pm 0.002	0.983 \pm 0.002	0.950 \pm 0.002
	1.022 \pm 0.003	1.052 \pm 0.002	0.998 \pm 0.002	1.001 \pm 0.002	1.040 \pm 0.002	0.980 \pm 0.002	0.951 \pm 0.002
Water							
Hole							
	1.069 \pm 0.002	1.076 \pm 0.002	Water	1.035 \pm 0.002	0.962 \pm 0.002	0.962 \pm 0.002	
	1.070 \pm 0.002	1.072 \pm 0.002	Hole	1.042 \pm 0.002	0.962 \pm 0.002	0.967 \pm 0.002	
	1.065 \pm 0.002	1.079 \pm 0.002		1.038 \pm 0.002			
Water							
Hole							
	1.047 \pm 0.003	1.090 \pm 0.002	1.080 \pm 0.002	0.992 \pm 0.002	0.962 \pm 0.002	0.962 \pm 0.002	
	1.048 \pm 0.003	1.095 \pm 0.002	1.081 \pm 0.002	0.994 \pm 0.002	0.962 \pm 0.002	0.962 \pm 0.002	
	1.050 \pm 0.003	1.094 \pm 0.002	1.081 \pm 0.002	0.993 \pm 0.002	0.967 \pm 0.002		
Water							
Hole							
	1.060 \pm 0.002	1.053 \pm 0.002	1.053 \pm 0.002	0.974 \pm 0.002	0.947 \pm 0.002	0.947 \pm 0.002	
	1.058 \pm 0.002	1.058 \pm 0.002	1.058 \pm 0.002	0.971 \pm 0.002	0.950 \pm 0.002	0.950 \pm 0.002	
				0.969 \pm 0.002	0.945 \pm 0.002	0.945 \pm 0.002	
Water							
Hole							
	0.990 \pm 0.003	0.952 \pm 0.002	0.952 \pm 0.002	0.944 \pm 0.002	0.944 \pm 0.002	0.944 \pm 0.002	
	0.987 \pm 0.003	0.949 \pm 0.002	0.949 \pm 0.002	0.941 \pm 0.002	0.941 \pm 0.002	0.941 \pm 0.002	
	0.990 \pm 0.003	0.954 \pm 0.002	0.954 \pm 0.002	0.942 \pm 0.002			
Water							
Hole							
	0.943 \pm 0.003	0.938 \pm 0.002	0.938 \pm 0.002	0.939 \pm 0.003	0.932 \pm 0.003	0.932 \pm 0.003	
	0.939 \pm 0.003	0.936 \pm 0.002	0.936 \pm 0.002	0.941 \pm 0.003	0.934 \pm 0.003	0.934 \pm 0.003	
	0.941 \pm 0.003						
ENDF/B-V							
ENDF/B-VI.2							
ENDF/B-VI.3							

Figure 3. Assembly Pin Power Distribution for Infinite-Lattice Configuration B.

Water	1.135 \pm 0.004	1.018 \pm 0.003	1.007 \pm 0.003	1.002 \pm 0.003	0.999 \pm 0.003	1.039 \pm 0.003	1.067 \pm 0.004
Hole	1.131 \pm 0.004	1.015 \pm 0.003	1.004 \pm 0.003	1.001 \pm 0.003	1.001 \pm 0.003	1.036 \pm 0.003	1.066 \pm 0.004
	1.137 \pm 0.004	1.016 \pm 0.003	1.009 \pm 0.003	1.000 \pm 0.003	1.003 \pm 0.003	1.037 \pm 0.003	1.059 \pm 0.004
	1.037 \pm 0.003	0.932 \pm 0.002	0.968 \pm 0.002	0.963 \pm 0.002	0.932 \pm 0.002	1.006 \pm 0.002	1.056 \pm 0.003
	1.038 \pm 0.003	0.932 \pm 0.002	0.969 \pm 0.002	0.963 \pm 0.002	0.932 \pm 0.002	1.010 \pm 0.002	1.058 \pm 0.003
	1.037 \pm 0.003	0.930 \pm 0.002	0.968 \pm 0.002	0.964 \pm 0.002	0.930 \pm 0.002	1.005 \pm 0.002	1.054 \pm 0.003
Pyrex		0.874 \pm 0.002	0.868 \pm 0.002			0.948 \pm 0.002	1.047 \pm 0.002
Rod		0.874 \pm 0.002	0.869 \pm 0.002	Pyrex		0.944 \pm 0.002	1.049 \pm 0.002
		0.876 \pm 0.002	0.870 \pm 0.002	Rod		0.943 \pm 0.002	1.043 \pm 0.002
		0.893 \pm 0.003	0.849 \pm 0.002	0.882 \pm 0.002	1.007 \pm 0.002	1.073 \pm 0.003	
		0.895 \pm 0.003	0.851 \pm 0.002	0.883 \pm 0.002	1.008 \pm 0.002	1.063 \pm 0.003	
		0.891 \pm 0.003	0.848 \pm 0.002	0.881 \pm 0.002	1.006 \pm 0.002	1.068 \pm 0.003	
				Pyrex		1.043 \pm 0.002	1.086 \pm 0.003
				Rod		1.046 \pm 0.002	1.087 \pm 0.003
						1.047 \pm 0.002	1.089 \pm 0.003
				1.022 \pm 0.003	1.081 \pm 0.002	1.105 \pm 0.003	
				1.022 \pm 0.003	1.086 \pm 0.002	1.105 \pm 0.003	
				1.020 \pm 0.003	1.086 \pm 0.002	1.113 \pm 0.003	
				1.113 \pm 0.003	1.125 \pm 0.003		
					1.109 \pm 0.003	1.128 \pm 0.003	
					1.117 \pm 0.003	1.129 \pm 0.003	
						ENDF/B-V	1.135 \pm 0.004
						ENDF/B-VI.2	1.137 \pm 0.004
						ENDF/B-VI.3	1.138 \pm 0.004

Figure 4. Assembly Pin Power Distribution for Infinite-Lattice Configuration C.