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Author(s):

R. D. Mosteller

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**HELIOS CALCULATIONS FOR  
UO<sub>2</sub> LATTICE BENCHMARKS**

Russell D. Mosteller

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

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## HELIOS CALCULATIONS FOR $\text{UO}_2$ LATTICE BENCHMARKS

Calculations for the ANS  $\text{UO}_2$  lattice benchmark<sup>1</sup> have been performed with the HELIOS lattice-physics code<sup>2</sup> and six of its cross-section libraries. The results obtained from the different libraries permit conclusions to be drawn regarding the adequacy of the energy group structures and of the ENDF/B-VI evaluation for  $^{238}\text{U}$ .

Scandpower A/S, the developer of HELIOS, provided Los Alamos National Laboratory with six different cross section libraries. Three of the libraries were derived directly from Release 3 of ENDF/B-VI (ENDF/B-VI.3) and differ only in the number of groups (34, 89 or 190). The other three libraries are identical to the first three except for a modification<sup>3</sup> to the cross sections for  $^{238}\text{U}$  in the resonance range.

Each of the fuel-pin and water-hole cells contain eight mesh regions. The fuel-pin cells contain two mesh regions in the fuel pin, one in the cladding, and five in the moderator. This mesh structure, although unconventional, was shown to accurately reproduce pin-cell results for much finer mesh structures (25 mesh regions in the fuel, one in the clad, and eight in the moderator). It was found that the introduction of an inner annulus in the moderator, producing a fifth mesh region in the water, was necessary to match pin-cell results from the MCNP Monte Carlo code.<sup>4</sup> The additional mesh region in the moderator is necessary because of the density of the water (approximately 50% more dense than at reactor operating conditions), as has been noted elsewhere.<sup>5</sup> Water-hole cells contain exactly the same mesh structure as the fuel-pin cells, although each mesh region contains only borated water.

In contrast, cells with Pyrex absorber rods each contain 20 mesh regions, 15 in the absorber rod and 5 in the moderator (the absorber rods have no cladding). The fine mesh structure in the absorber pins was chosen because of differences in results between HELIOS and MCNP. However, as will be discussed later, the HELIOS results are quite insensitive to the number of mesh regions in the absorber rods.

The HELIOS calculations were performed with collision-probability calculations for the individual pin cells, and the pin cells were coupled using cosine currents. A few of the infinite-lattice cases were run using collision probabilities for the entire assembly, but the difference in  $k_{\infty}$  relative to the corresponding cases with cosine-current coupling was negligible. The input buckling was  $0.00037 \text{ cm}^{-2}$  for the core cases and zero for the infinite-lattice cases.

The results for the core configurations are given in Table 1. Core calculations were performed only with the 89-group and 34-group libraries because of storage limitations imposed by the computer system employed. Table 1 also includes corresponding results<sup>6</sup> from MCNP with continuous-energy cross sections derived from ENDF/B-VI.3. Comparisons amongst the HELIOS results can quantify the effect of the number of energy groups and of the modification to the  $^{238}\text{U}$  cross sections, while comparisons between the results from HELIOS and MCNP permit methodological effects to be separated from cross-section effects.

The 89-group library with the modified  $^{238}\text{U}$  cross sections produces better agreement with the benchmark value for  $k_{\text{eff}}$  ( $1.0007 \pm 0.0006$ ) than does the 89-group library with true ENDF/B-VI.3 cross sections. However, the 89-group ENDF/B-VI.3 library produces much better agreement with the MCNP values for  $k_{\text{eff}}$ . This result suggests that the modification produces more accurate behavior for  $^{238}\text{U}$  and that the ENDF/B-VI.3 evaluation for  $^{238}\text{U}$  may need to be modified accordingly.

Two other trends also are evident from Table 1. First, the 34-group library consistently predicts a value for  $k_{\text{eff}}$  that is approximately  $0.003 \Delta k$  higher than that from the corresponding 89-group library. Second, all four libraries predict a downward swing of approximately  $0.005 \Delta k$  between core B and core C. Although MCNP also predicts a downward swing, the magnitude of that swing is less than  $0.002 \Delta k$ .

Calculations for the infinite-lattice configurations were performed with all six cross-section libraries. In general, the 190-group libraries produce results that are very similar to those from the corresponding 89-group libraries. In addition, all six libraries produce virtually identical pin power distributions for the infinite-lattice configurations.

Not surprisingly, the same reactivity trends that are observed for the core configurations also are present in the results for the infinite-lattice configurations, as Table 2 shows. In particular, the ENDF/B-VI.3 190-group and 89-group libraries produce results in good agreement with MCNP, all six libraries produce a much bigger reactivity swing between lattices A and B than MCNP does, and the 34-group libraries consistently overpredict  $k_{\infty}$  relative to the corresponding 190-group and 89-group libraries.

The results for the spectral indices also provide insight into the higher value of  $k_{\infty}$  predicted by the 34-group libraries. The 34-group library produces essentially the same values for  $\delta_{25}$  (fast-to-thermal fission ratio in  $^{235}\text{U}$ ) and  $\rho_{28}$  (fast-to-thermal capture ratio in  $^{238}\text{U}$ ) as does the 190-group library. However, it produces lower values for  $\delta_{28}$  (ratio of fissions in  $^{238}\text{U}$  to fissions in  $^{235}\text{U}$ ) and the conversion ratio (CR) and higher values for  $\rho_{25}$  (fast-to-thermal capture ratio in  $^{235}\text{U}$ ). Taken together, these results suggest that the 34-group library produces slightly more fissions and slightly fewer thermal captures in  $^{235}\text{U}$ . Both of these differences tend to increase  $k_{\infty}$ .

The larger reactivity swing between lattices B and C predicted by HELIOS relative to MCNP is due almost to the difference in the Pyrex absorption fraction (PAF). We have not been able to determine the cause for this behavior, however. For example, the value for  $k_{\text{eff}}$  with 5 mesh regions in the Pyrex is only  $0.00001 \Delta k$  less than the value with 15. It is possible, although unlikely, that some problem exists with the boron cross sections, since HELIOS predicts about the same value for  $k_{\text{eff}}$  as MCNP for cases with assembly A (1511 PPM) but a slightly higher value for cases with assembly B (1335.5 PPM).

Some additional insight can be gained by comparing the spectral indices from HELIOS with those from MCNP. HELIOS consistently predicts slightly higher values for  $\delta_{25}$  and  $\rho_{25}$ , which indicates that it tends to predict a harder spectrum. However, a harder spectrum also should produce larger values for  $\delta_{28}$  and  $\rho_{28}$ , whereas HELIOS actually predicts lower values for

those indices than MCNP (the exception,  $p_{28}$  for infinite-lattice configuration C, probably results from the harder spectrum induced by the higher capture rate in the Pyrex). An alternative explanation is that the HELIOS libraries predict less absorption in  $^{238}\text{U}$ , and this suspicion is reinforced by the fact that HELIOS produces lower conversion ratios than MCNP. All in all, the HELIOS ENDF/B-VI.3 libraries appear to produce slightly higher absorption rates in  $^{235}\text{U}$  and lower absorption rates in  $^{238}\text{U}$  than the MCNP library does.

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Table 1. Reactivity Results for Core Configurations.

Core	$k_{\text{eff}}$ , MCNP	HELIOS Library		$k_{\text{eff}}$ , HELIOS
		Groups	<sup>238</sup> U	
A	$0.9956 \pm 0.0003$	89	ENDF/B-VI.3	0.9956
			Modified	0.9992
		34	ENDF/B-VI.3	0.9988
			Modified	1.0025
B	$0.9957 \pm 0.0003$	89	ENDF/B-VI.3	0.9971
			Modified	1.0004
		34	ENDF/B-VI.3	1.0005
			Modified	1.0038
C	$0.9940 \pm 0.0003$	89	ENDF/B-VI.3	0.9917
			Modified	0.9951
		34	ENDF/B-VI.3	0.9942
			Modified	0.9977



Table 2. Results for Infinite-Lattice Configurations.

Lattice	Index	MCNP	HELIOS (ENDF/B-VI.3)				HELIOS ( $^{238}\text{U}$ Modified)			
			190 Groups	89 Groups	34 Groups	190 Groups	89 Groups	34 Groups	190 Groups	89 Groups
A	$k_{\infty}$	$1.0582 \pm 0.0003$	1.0575	1.0566	1.0592	1.0614	1.0639	1.0631	1.0614	1.0639
	$\delta_{25}$	$0.1297 \pm 0.0001$	0.1306	0.1308	0.1309	0.1305	0.1307	0.1308	0.1305	0.1307
	$\delta_{28}$	$0.0649 \pm 0.0001$	0.0622	0.0622	0.0616	0.0620	0.0620	0.0613	0.0620	0.0620
	$\rho_{25}$	$0.3619 \pm 0.0004$	0.3736	0.3786	0.3802	0.3735	0.3785	0.3801	0.3735	0.3785
	$\rho_{28}$	$2.2923 \pm 0.0024$	2.2441	2.2559	2.2461	2.1896	2.2020	2.1906	2.1896	2.2020
	CR	$0.4710 \pm 0.0004$	0.4620	0.4633	0.4619	0.4543	0.4557	0.4540	0.4543	0.4557
B	$k_{\infty}$	$1.0466 \pm 0.0003$	1.0500	1.0497	1.0526	1.0534	1.0530	1.0561	1.0534	1.0530
	$\delta_{25}$	$0.1153 \pm 0.0001$	0.1164	0.1166	0.1166	0.1163	0.1165	0.1165	0.1163	0.1165
	$\delta_{28}$	$0.0601 \pm 0.0001$	0.0580	0.0580	0.0575	0.0578	0.0578	0.0573	0.0578	0.0578
	$\rho_{25}$	$0.3211 \pm 0.0003$	0.3338	0.3379	0.3391	0.3337	0.3378	0.3390	0.3337	0.3378
	$\rho_{28}$	$2.0448 \pm 0.0023$	2.0363	2.0399	2.0285	1.9884	1.9926	1.9799	1.9884	1.9926
	CR	$0.4414 \pm 0.0003$	0.4381	0.4383	0.4367	0.4312	0.4315	0.4297	0.4312	0.4315
C	$k_{\infty}$	$0.9842 \pm 0.0003$	0.9798	0.9795	0.9811	0.9831	0.9828	0.9845	0.9831	0.9828
	$\delta_{25}$	$0.1282 \pm 0.0001$	0.1308	0.1310	0.1312	0.1307	0.1309	0.1311	0.1307	0.1309
	$\delta_{28}$	$0.0658 \pm 0.0001$	0.0639	0.0639	0.0635	0.0637	0.0637	0.0632	0.0637	0.0637
	$\rho_{25}$	$0.3585 \pm 0.0004$	0.3757	0.3803	0.3822	0.3756	0.3802	0.3821	0.3756	0.3802
	$\rho_{28}$	$2.2859 \pm 0.0025$	2.2967	2.3009	2.2909	2.2420	2.2470	2.2354	2.2420	2.2470
	CR	$0.4700 \pm 0.0004$	0.4687	0.4689	0.4675	0.4610	0.4613	0.4597	0.4610	0.4613
	PAF	$0.1389 \pm 0.0002$	0.1423	0.1422	0.1424	0.1420	0.1427	0.1429	0.1420	0.1427