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HELIOS CALCULATIONS FOR UO_2 LATTICE BENCHMARKS

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ABSTRACT

Calculations for the ANS UO_2 lattice benchmark have been performed with the HELIOS lattice-physics code and six of its cross-section libraries derived from ENDF/B-VI Release 3. The results obtained from these comparisons suggest that further refinement may be needed to the cross sections for ^{238}U. They also suggest that different group structures among the libraries produce a small but consistent reactivity bias.

I. INTRODUCTION

Los Alamos National Laboratory (LANL) initially purchased the HELIOS lattice-physics code[1] from Scandpower A/S several years ago, along with a set of cross-section libraries based on Release 2 of ENDF/B-VI. Subsequently, Scandpower provided LANL with six additional cross- section libraries. Three of the latter 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[2] to the cross sections for ^{238}U in the resonance range.

HELIOS solves the two-dimensional neutron transport equation using the method of collision probabilities (CPs). At the user's option, adjacent regions can be coupled neutronically using cosine-current coupling (CCC) rather than CPs.

II. BENCHMARK MODELS

HELIOS calculations have been performed with all six libraries for the ANS UO_2 lattice benchmark.[3] Fluxes within individual pin cells were calculated with CPs, and adjacent pin cells were coupled using CCC. A few of the infinite-lattice cases were run using CPs for the entire assembly, but, as shown in Table I, the difference in k_∞ relative to the corresponding cases with CCCs is essentially negligible.

Table I
Comparison of CCC versus CP Results
for Infinite-Lattice Cases

Configuration	Groups	k_∞	
		CCC	CP
B	190	1.0500	1.0503
C	190	0.9798	0.9806
C	89	0.9795	0.9798

Each of the fuel-pin cells contains eight mesh regions: two 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 presence of an inner annulus in the moderator was necessary to match pin-cell results from the MCNP Monte Carlo code.[4] The finer mesh 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.[5] Water-hole cells contain exactly the same mesh structure as the fuel-pin cells, although each mesh region contains only borated water.

Cells with Pyrex absorber rods each contain seven mesh regions, two in the absorber rod and five in the moderator (the absorber rods have no cladding). Much finer mesh structures, with as many as 25 mesh regions in the absorber pins, were investigated because of differences in results between HELIOS and MCNP. However, it was found that the HELIOS results are quite insensitive to the number of mesh regions in the absorber rods.

III. RESULTS FOR CORE CONFIGURATIONS

The results for the core configurations are given in Table II. An input buckling of 0.00037 cm^{-2} was used for these cases. Core calculations were performed only with the 89-group and 34-group libraries because of storage limitations imposed by the computer system employed. Table II also includes corresponding results[6] from MCNP calculations 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}U cross sections, while comparisons between the ENDF/B-VI.3 results from HELIOS and MCNP permit methodological effects to be separated from cross-section effects.

The 89-group library with the modified ^{238}U cross sections produces better agreement with the benchmark value for k_{eff} (1.0007 ± 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_{eff}. This result suggests that the modification to ^{238}U produces more accurate behavior and that the ENDF/B-VI.3 evaluation for ^{238}U may need to be modified accordingly.

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

Pin-power distributions for the central assembly in cores B and C are shown in Figures 1 and 2. Although the results are shown only for the true ENDF/B-VI.3 libraries, the distributions from the modified libraries are effectively identical.

IV. RESULTS FOR INFINITE-LATTICE CONFIGURATIONS

Calculations for the infinite-lattice configurations were performed with all six cross-section libraries. 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 III shows. In particular, the true ENDF/B-VI.3 190-group and 89-group libraries produce results in good agreement with MCNP,and all six libraries produce much bigger reactivity swings between lattices A and B than MCNP does. Although the 190-group libraries produce results that are very similar to those from the corresponding 89-group libraries, the 34-group libraries consistently predict a value for k_∞ that is approximately 0.003 Δk higher. All six for k_∞ that is libraries produce effectively identical pin-power distributions. However, as shown in Figures 3 and 4,those distributions differ slightly from the distributions predicted by MCNP.

Table II
Reactivity Results for Core Configurations

Core	k_{eff}, MCNP	HELIOS Library		k_{eff}, HELIOS
		Groups	^{238}U	
A	0.9956 ± 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 ± 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 ± 0.0003	89	ENDF/B-VI.3	0.9917
			Modified	0.9951
		34	ENDF/B-VI.3	0.9942
			Modified	0.9977

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

The larger reactivity swing between lattices B and C predicted by HELIOS relative to MCNP is due almost entirely to the difference in the Pyrex absorption fraction (PAF). Although the cause for this behavior has not been determined, it does not appear to be related to the mesh structure for the absorber pin. For example, the value for k_∞ with two mesh regions in the Pyrex is only 0.0003 Δk 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 reactivity as MCNP for cases with assembly A (1511 PPM) but slightly greater values 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 δ_{25} and ρ_{25}, which suggests that it may predict a harder spectrum. However, a harder spectrum also should produce larger values for δ_{28} and ρ_{28}, whereas HELIOS actually predicts lower values for those indices than MCNP (the exception, ρ_{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}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}U and lower absorption rates in ^{238}U than the MCNP library does.

IV. CONCLUSIONS

All six libraries produce reasonable agreement with the benchmarks. Two additional conclusions can be drawn from the results presented herein.

First, the modified 89-group HELIOS library consistently produces better agreement in reactivity with the core benchmarks than does its true ENDF/B-VI.3 counterpart. However, the ENDF/B-VI.3 libraries consistently produce better agreement with MCNP results than the modified libraries. This pattern suggests that the ENDF/B-VI.3 representation for ^{238}U may need to be modified.

Second, the 34-group libraries consistently produce a bias of approximately 0.003 Δk relative to the 89- and 190-group libraries. The principal cause of this bias appears to be the cross sections for ^{235}U.

REFERENCES

1. Eduardo Villarino, Rudi J. J. Stamm'ler, Aldo Ferri, and Juan J. Casal, "HELIOS: Angularly Dependent Collision Probabilities," *Nucl. Sci. Eng.*, **112**, pp. 16–31 (September 1992).

2. M. Edenius, "Adjustment of the Effective ^{238}U Resonance Integral to Force Agreement with Integral Data," pp. 87-94, *Seminar on ^{238}U Resonance Capture*, S. Pearlstein, Ed., BNL-NCS-50451 (CONF-750323) (March 1975).

3. Theodore A. Parish, David J. Diamond, Russell D. Mosteller, and Jess C. Gehin, "Summary of Results For the Uranium Benchmark Problem of the ANS *Ad Hoc* Committee on Reactor Physics Benchmarks," presented at the International Conference on the Physics of Nuclear Science and Technology (October 5-8, 1998, Islandia, Long Island, New York).

4. Judith F. Briesmeister, Ed., "MCNP—A General Monte Carlo N-Particle Transport Code, Version 4B," Los Alamos National Laboratory report LA-12625-M, Version 4B (March 1997).

5. W. J. Eich, O. Ozer, and R. D. Mosteller, "Cell Criticals Benchmarking," Part I, Chapter 2, *ARMP-02 Documentation*, Electric Power Research Institute report NP-4574-CCM (August 1988).

6. Russell D. Mosteller, "ENDF/B-V and ENDF/B-VI Results for UO_2 Lattice Benchmark Problems Using MCNP," presented at the International Conference on the Physics of Nuclear Science and Technology (October 5-8, 1998, Islandia, Long Island, New York).

Water Hole	1.107±0.002 1.109 1.109 1.119±0.013	1.026±0.006 1.058 1.058 1.059±0.012	1.000±0.001 1.036 1.036 1.017±0.011	1.025±0.007 1.027 1.027 1.028±0.012	1.026±0.003 1.024 1.024 1.021±0.012	0.980±0.021 1.000 1.000 0.978±0.011	0.983±0.008 0.976 0.976 0.963±0.011
	1.068±0.002 1.091 1.091 1.072±0.012	1.075±0.000 1.101 1.101 1.107±0.009	1.036±0.007 1.061 1.061 1.051±0.009	1.047±0.004 1.054 1.054 1.047±0.009	1.098±0.006 1.073 1.073 1.070±0.009	1.026±0.023 1.020 1.020 1.013±0.009	1.003±0.031 0.981 0.981 0.969±0.008
		Water Hole	1.116±0.012 1.113 1.113 1.113±0.009	1.118±0.011 1.111 1.111 1.139±0.009	Water Hole	1.070±0.010 1.060 1.060 1.073±0.009	0.961±0.010 0.987 0.987 0.984±0.008
			1.091±0.009 1.103 1.103 1.097±0.012	1.145±0.008 1.129 1.129 1.148±0.009	1.133±0.010 1.107 1.107 1.135±0.009	1.032±0.026 1.026 1.026 1.030±0.008	0.924±0.006 0.979 0.979 0.972±0.008
				Water Hole	1.109±0.007 1.079 1.079 1.095±0.009	1.007±0.014 0.998 0.998 1.003±0.008	0.974±0.026 0.966 0.966 0.953±0.008
					1.015±0.002 1.018 1.018 1.019±0.012	0.973±0.023 0.975 0.974 0.976±0.008	0.971±0.012 0.953 0.953 0.944±0.008
						0.970±0.006 0.955 0.955 0.932±0.011	0.950±0.005 0.941 0.941 0.937±0.008
						Measured HELIOS, 89 Groups HELIOS, 34 Groups MCNP	0.920±0.013 0.931 0.930 0.934±0.011

RMS Differences

89 Groups	34 Groups	MCNP
0.021	0.021	0.019

Figure 1. Pin Power Distributions in Central Assembly of Core B (ENDF/B-VI.3 Libraries).

Water Hole	1.148±0.007 1.125 1.124 1.144±0.019	1.027±0.004 1.034 1.033 1.048±0.017	1.045±0.006 1.022 1.022 1.021±0.016	1.057±0.006 1.025 1.025 1.034±0.017	1.047±0.005 1.033 1.033 1.009±0.016	1.088±0.004 1.071 1.071 1.106±0.017	1.124±0.016 1.104 1.104 1.114±0.017
	1.036±0.005 1.052 1.051 1.069±0.018	0.945±0.007 0.966 0.965 0.957±0.012	1.001±0.006 0.986 0.985 0.967±0.012	0.982±0.021 0.989 0.989 0.985±0.012	0.962±0.008 0.972 0.972 0.958±0.012	1.070±0.014 1.044 1.044 1.050±0.012	1.105±0.009 1.099 1.099 1.099±0.009
		Pyrex Rod	0.901±0.006 0.916 0.915 0.902±0.011	0.900±0.019 0.917 0.916 0.890±0.011	Pyrex Rod	1.001±0.021 0.999 0.999 1.005±0.012	1.087±0.007 1.094 1.095 1.097±0.012
			0.914±0.004 0.920 0.919 0.938±0.016	0.854±0.017 0.895 0.895 0.878±0.011	0.933±0.005 0.933 0.933 0.912±0.011	1.049±0.014 1.045 1.045 1.033±0.012	1.088±0.005 1.112 1.113 1.122±0.012
				Pyrex Rod	0.970±0.006 0.981 0.981 0.954±0.011	1.097±0.020 1.093 1.093 1.105±0.012	1.138±0.015 1.139 1.139 1.146±0.013
					1.071±0.006 1.068 1.068 1.087±0.017	1.140±0.014 1.135 1.135 1.145±0.013	1.195±0.006 1.166 1.167 1.173±0.013
						1.164±0.003 1.168 1.169 1.181±0.018	1.199±0.008 1.188 1.190 1.209±0.013
						Measured HELIOS, 89 Groups HELIOS, 34 Groups MCNP	1.206±0.011 1.203 1.205 1.238±0.018

RMS Differences

89 Groups	34 Groups	MCNP
0.017	0.018	0.019

Figure 2. Pin Power Distributions in Central Assembly of Core C (ENDF/B-VI.3 Libraries).

Table III
Results for Infinite-Lattice Configurations

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

Water Hole	1.048 1.048 1.048 1.054 ± 0.004	1.002 1.002 1.002 0.996 ± 0.003	0.984 0.984 0.984 0.972 ± 0.003	0.980 0.980 0.980 0.971 ± 0.003	0.982 0.982 0.982 0.978 ± 0.003	0.966 0.966 0.966 0.959 ± 0.003	0.951 0.951 0.951 0.944 ± 0.003
	1.032 1.032 1.032 1.022 ± 0.003	1.043 1.044 1.044 1.052 ± 0.002	1.008 1.009 1.009 0.998 ± 0.002	1.006 1.007 1.007 1.001 ± 0.002	1.030 1.030 1.031 1.040 ± 0.002	0.987 0.987 0.987 0.980 ± 0.002	0.957 0.957 0.957 0.951 ± 0.002
		Water Hole	1.059 1.060 1.060 1.065 ± 0.002	1.062 1.063 1.063 1.079 ± 0.002	Water Hole	1.026 1.026 1.026 1.038 ± 0.002	0.965 0.964 0.965 0.967 ± 0.002
			1.054 1.054 1.054 1.050 ± 0.003	1.083 1.084 1.084 1.094 ± 0.002	1.068 1.068 1.068 1.081 ± 0.002	0.997 0.997 0.997 0.993 ± 0.002	0.960 0.960 0.960 0.967 ± 0.002
				Water Hole	1.045 1.045 1.045 1.058 ± 0.002	0.974 0.974 0.974 0.969 ± 0.002	0.951 0.951 0.951 0.945 ± 0.002
					0.992 0.992 0.992 0.990 ± 0.003	0.957 0.957 0.957 0.954 ± 0.002	0.944 0.944 0.944 0.942 ± 0.002
						0.945 0.944 0.944 0.941 ± 0.003	0.939 0.939 0.939 0.934 ± 0.002
						HELIOS, 190 Groups HELIOS, 89 Groups HELIOS, 34 Groups MCNP	0.937 0.937 0.936 0.937 ± 0.003

Figure 3. Assembly Pin Power Distribution for Infinite-Lattice Configuration B (ENDF/B-VI.3 Libraries).

Water Hole	1.099 1.099 1.098 1.137 ± 0.004	1.008 1.008 1.008 1.016 ± 0.003	0.995 0.995 0.994 1.009 ± 0.003	0.994 0.994 0.994 1.000 ± 0.003	0.998 0.998 0.998 1.003 ± 0.003	1.028 1.028 1.028 1.037 ± 0.003	1.054 1.054 1.054 1.059 ± 0.004
	1.027 1.027 1.026 1.037 ± 0.003	0.942 0.942 0.942 0.930 ± 0.002	0.959 0.959 0.959 0.968 ± 0.002	0.959 0.959 0.959 0.964 ± 0.002	0.939 0.939 0.939 0.930 ± 0.002	1.002 1.002 1.002 1.005 ± 0.002	1.049 1.049 1.049 1.054 ± 0.003
		Pyrex Rod	0.890 0.890 0.889 0.876 ± 0.002	0.888 0.888 0.888 0.870 ± 0.002	Pyrex Rod	0.958 0.958 0.958 0.943 ± 0.002	1.044 1.044 1.044 1.043 ± 0.002
			0.892 0.892 0.891 0.891 ± 0.003	0.865 0.865 0.865 0.848 ± 0.002	0.897 0.897 0.897 0.881 ± 0.002	1.000 1.000 1.000 1.006 ± 0.002	1.059 1.059 1.059 1.068 ± 0.003
				Pyrex Rod	0.941 0.941 0.941 0.924 ± 0.002	1.043 1.043 1.044 1.047 ± 0.002	1.082 1.082 1.082 1.089 ± 0.003
					1.021 1.021 1.021 1.020 ± 0.003	1.080 1.080 1.080 1.086 ± 0.002	1.105 1.105 1.105 1.113 ± 0.003
						1.108 1.108 1.108 1.117 ± 0.003	1.122 1.122 1.123 1.129 ± 0.003
						HELIOS, 190 Groups HELIOS, 89 Groups HELIOS, 34 Groups MCNP	1.132 1.132 1.132 1.138 ± 0.004

Figure 4. Assembly Pin Power Distribution for Infinite-Lattice Configuration C (ENDF/B-VI.3 Libraries).