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Comparison of Results for the MCNP Criticality Validation Suite Using ENDF/B-VII and Other Nuclear Data Libraries

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Abstract

The latest pre-release version of ENDF/B-VII ("ENDF/B-VII β-2") was made available for testing in April 2006. Calculations were performed for the 31 cases in the MCNP Criticality Validation Suite for ENDF/B-VII β-2, its predecessors ENDF/B-VII β-1 and ENDF/B-VI, and JENDL-3.3. Overall, β-2 produces results similar to β-1, but it produces substantially improved results relative to ENDF/B-VI and JENDL-3.3. However, calculations for some additional benchmarks indicate that further improvements still are needed in certain areas.

KEYWORDS: ENDF/B-VII, ENDF/B-VI, JENDL-3.3, criticality, benchmarks, MCNP, Criticality Validation Suite

1. Overview

A pre-release version of ENDF/B-VII ("ENDF/B-VII β-2") was made available for testing in April 2006. The previous pre-release version, ENDF/B-VII β-1, had been made available about six months earlier. Calculations for the 31 cases in the MCNP Criticality Validation Suite have been performed with those two libraries and two others, ENDF/B-VI and JENDL-3.3, to assess the reactivity impact of the changes to nuclear data incorporated into ENDF/B-VII β-2. The results from those calculations, in combination with those from a number of other cases specifically selected to illustrate known or suspected deficiencies in the data, permit an assessment of areas where improvements have occurred or are still needed.

2. ENDF/B-VII Nuclear Data

Many changes and additions to nuclear data have been made for ENDF/B-VII β-1 and β-2, but a subset of those changes is most important for the criticality benchmarks studied herein. Significant changes were made to most of the actinides, and changes were made to the (n,α) cross section for ^{16}O and to the thermal capture cross section for ^{1}H as well. In addition, a number of elemental evaluations were replaced with isotopic ones, and some new thermal scattering data were added. However, these latter changes lead to fairly small criticality effects.

Substantive changes were made for the principal uranium isotopes and for ^{232}Th. The ^{235}U fission cross section was increased in the MeV range. Because the cross sections of many actinides

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are measured with respect to ^{235}U, this revision caused the fission cross sections for plutonium and other actinides to increase as well. In addition, a completely new and modern evaluation for ^{233}U was prepared with emphasis on a good treatment of elastic and inelastic scattering. Changes also were made to the elastic and inelastic scattering cross sections for ^{238}U, and a new ^{232}Th evaluation was provided by the IAEA. New evaluations of the resonance parameters for ^{233}U, ^{235}U, and ^{238}U also were included, and a number of additional changes were made for the minor actinides.

The change to ^{1}H propagated to a number of other materials, because it also is used as a standard. The thermal scattering law for hydrogen in light water also was revised. This change has little reactivity impact for large solution benchmarks, but it can increase k_{eff} for lattices and high-leakage thermal benchmarks by 0.0010 to 0.0025 Δk. The increase in the (n,α) cross section for ^{16}O is expected to increase reactivity by approximately 0.0010 Δk for benchmarks that contain large amounts of oxygen.

3. The MCNP Criticality Validation Suite

The MCNP criticality validation suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments* [1]. The cases in the suite were selected to encompass a variety of fissile materials in configurations that produce fast, intermediate, and thermal spectra. The selected benchmarks include cases with highly enriched uranium (HEU), intermediate enriched uranium (IEU), low enriched uranium (LEU), ^{233}U, and plutonium. The suite includes cases with fast, intermediate, and thermal spectra for each fuel type except LEU, which of course can achieve criticality only with a thermal spectrum. The distribution of cases by fuel material and spectrum is shown in Table 1, and a brief summary of each case is provided in Table 2.

4. Calculations and Results

Four sets of calculations were performed for the suite using the MCNP5 Monte Carlo code [2]. The first set employed a nuclear data library derived derived from JENDL-3.3 [3]. The second set employed nuclear data from ENDF/B-VI Release 8, the final release for ENDF/B-VI. The third set employed ENDF/B-VII β-1, and the fourth set used ENDF/B-VII β-1. The SAB2002 library [4] of thermal scattering laws, S(α,β), was used where needed for the JENDL-3.3 and ENDF/B-VI calculations, and ENDF/B-VI data were used in the ENDF/B-VII calculations for those few instances where ENDF/B-VII data were not readily available (e.g., gold, ^{232}U).

The MCNP5 calculations were run with 5,000,000 active neutron histories for all but two cases in the suite. Only 3,000,000 active histories were used for those cases, SB-5 and Zebra-8H, because they require substantially more computer time per history than the other cases. Nonetheless, the standard deviation for k_{eff} from those cases is comparable to those from other cases in the suite. This number of histories is sufficient to render the statistical uncertainty from the MCNP5 calculations essentially negligible relative to the benchmark uncertainty for most of the cases in the suite.

The results from these calculations are presented in Tables 3 and 4. ENDF/B-VII β-1 and β-2 produce very similar results, with only a few exceptions. β-2 produces slightly higher values of k_{eff} for almost all of the benchmarks that involve water, although the size of the increase varies from case to case. These differences are due primarily to the changes in the (n,α) cross section for ^{16}O and in the scattering law for hydrogen in water.

Table 1: MCNP Criticality Validation Suite.

Spectrum	Fast			Intermediate	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins in Water	Solution
HEU	Godiva Tinkertoy-2 (c-11)*	Flattop-25	Godiver	UH_3 (6) Zeus (2)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H‡	IEU-CT-02 (3)	STACY (36)
LEU					BaW XI (2)	LEU-ST-02 (2)
^{233}U	Jezebel-233	Flattop-23	U233-MF-05 (2)	Falstaff (1)†	SB-2½	ORNL-11
Pu	Jezebel Jezebel-240 Pu Buttons (3)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG‡	PNL-33	PNL-2

* Numbers in parentheses identify a specific case within a sequence of benchmarks
‡ k_∞ measurement
† Extrapolated to critical

Table 2: Summary of cases in the MCNP criticality validation suite.

Case	Description
Godiva	Bare sphere of HEU
Tinkertoy-2 (c-11)	3 x 3 x 3 array of HEU cylinders reflected by paraffin
Flattop-25	Sphere of HEU reflected by normal uranium
Godiver	Sphere of HEU reflected by water
Zeus (2)	Cylinder of HEU plates moderated by graphite and reflected by copper
UH_3 (6)	Cylinder of HEU UH_3 cans reflected by depleted uranium
SB-5	Lattice of HEU pins in water surrounded by a blanket of ThO_2 pins
ORNL-10	Sphere of HEU uranyl nitrate solution
IEU-MF-03	Bare sphere of IEU (36 wt.%)
BIG TEN	Cylinder of IEU (10 wt.%) reflected by normal uranium
IEU-MF-04	Sphere of IEU (36 wt.%) reflected by graphite
Zebra-8H	Plate of IEU (37.5 wt.%) reflected by normal uranium and steel
IEU-CT-02 (3)	Lattice of IEU (17 wt.%) fuel rods in water
Stacy (36)	Cylinder of IEU (9.97 wt.%) uranyl nitrate solution
BaW LRC XI (2)	Lattice of LEU (2.46 wt.%) UO_2 fuel pins in borated water
LEU-ST-02 (2)	Sphere of LEU (4.9 wt.%) uranyl fluoride solution
Jezebel-233	Bare sphere of ^{233}U
Flattop-23	Sphere of ^{233}U reflected by normal uranium
U233-MF-05 (2)	Sphere of ^{233}U reflected by beryllium
Falstaff (1)	Sphere of ^{233}U uranyl fluoride solution
SB-2½	Lattice of ^{233}U fuel pins in water
ORNL-11	Sphere of ^{233}U uranyl nitrate solution
Jezebel	Bare sphere of plutonium
Jezebel-240	Bare sphere of plutonium (20.1 at.% ^{240}Pu)
Pu Buttons (3)	3 x 3 x 3 array of small cylinders of plutonium
Flattop-Pu	Plutonium sphere reflected by normal uranium
THOR	Plutonium sphere reflected by thorium
Pu-MF-11	Plutonium sphere reflected by water
HISS/HPG	Infinite, homogeneous mixture of plutonium, hydrogen, and graphite
PNL-33	Lattice of mixed-oxide fuel pins in borated water
PNL-2	Sphere of plutonium nitrate solution

Relative to ENDF/B-VI, ENDF/B-VII β-1 and β-2 produce substantial improvements for Jezebel, Jezebel-233 and Godiva, both individually and relative to the corresponding Flattop cases. In addition, the improvements for THOR and, especially, BIG TEN are particularly noteworthy. They also produce higher values of k_{eff} for many of the benchmarks that contain water, including thermal lattices and water-reflected metal spheres. The improvement for the LEU lattice is particularly striking, because it resolves a long-standing discrepancy. It is most likely due primarily to changes in the resonance parameters for the uranium isotopes.

Table 3: MCNP5 results for HEU, IEU, and LEU benchmarks in the Criticality Validation Suite.

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII β-2	ENDF/B-VII β-1	ENDF/B-VI	JENDFL-3.3
Godiva	1.0000 ± 0.0010	1.0004 ± 0.0003	0.9999 ± 0.0003	**0.9963 ± 0.0003**	**1.0033 ± 0.0003**
Tinkertoy-2 (c-11)	1.0000 ± 0.0038	1.0006 ± 0.0004	1.0006 ± 0.0003	0.9973 ± 0.0004	**1.0042 ± 0.0003**
Flattop-25	1.0000 ± 0.0030	**1.0034 ± 0.0003**	**1.0033 ± 0.0003**	1.0021 ± 0.0003	0.9974 ± 0.0003
Godiver	0.9985 ± 0.0011	**1.0005 ± 0.0004**	0.9988 ± 0.0004	**0.9948 ± 0.0003**	**1.0019 ± 0.0004**
UH_3 (6)	1.0000 ± 0.0047	0.9953 ± 0.0004	**0.9947 ± 0.0004**	**0.9914 ± 0.0003**	0.9967 ± 0.0004
Zeus (2)	0.9997 ± 0.0008	**0.9966 ± 0.0003**	**0.9963 ± 0.0003**	**0.9942 ± 0.0003**	**0.9956 ± 0.0003**
SB-5	1.0015 ± 0.0028	**0.9964 ± 0.0006**	**0.9959 ± 0.0005**	**0.9965 ± 0.0005**	0.9990 ± 0.0006
ORNL-10	1.0015 ± 0.0026	0.9996 ± 0.0002	**0.9987 ± 0.0002**	0.9992 ± 0.0002	0.9999 ± 0.0002
IEU-MF-03	1.0000 ± 0.0017	**1.0022 ± 0.0003**	**1.0030 ± 0.0003**	0.9987 ± 0.0003	**0.9969 ± 0.0002**
BIG TEN	0.9948 ± 0.0013	0.9952 ± 0.0002	0.9954 ± 0.0002	**1.0071 ± 0.0003**	**0.9851 ± 0.0002**
IEU-MF-04	1.0000 ± 0.0030	**1.0078 ± 0.0003**	**1.0075 ± 0.0003**	**1.0036 ± 0.0003**	1.0024 ± 0.0003
Zebra-8H	1.0300 ± 0.0025	**1.0189 ± 0.0002**	**1.0199 ± 0.0003**	**1.0406 ± 0.0002**	**1.0152 ± 0.0002**
IEU-CT-02 (3)	1.0017 ± 0.0044	1.0039 ± 0.0003	1.0002 ± 0.0003	1.0004 ± 0.0003	1.0014 ± 0.0003
STACY-36	0.9988 ± 0.0013	0.9989 ± 0.0003	0.9981 ± 0.0003	0.9986 ± 0.0003	0.9999 ± 0.0003
BaW XI (2)	1.0007 ± 0.0012	1.0012 ± 0.0003	1.0005 ± 0.0003	**0.9968 ± 0.0003**	**0.9991 ± 0.0003**
LEU-ST-02 (2)	1.0024 ± 0.0037	**0.9954 ± 0.0003**	**0.9951 ± 0.0003**	**0.9953 ± 0.0003**	**0.9963 ± 0.0003**

$\sigma < |\Delta k| \le 2\sigma$ **$|\Delta k| > 2\sigma$**

Table 4: MCNP5 results for the ^{233}U and plutonium benchmarks in the Criticality Validation Suite.

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII β-2	ENDF/B-VII β-1	ENDF/B-VI	JENDFL-3.3
Jezebel-233	1.0000 ± 0.0010	0.9996 ± 0.0003	0.9997 ± 0.0003	**0.9926 ± 0.0003**	**1.0041 ± 0.0003**
Flattop-23	1.0000 ± 0.0014	0.9990 ± 0.0003	0.9992 ± 0.0003	1.0003 ± 0.0003	0.9985 ± 0.0003
U233-MF-05 (2)	1.0000 ± 0.0030	0.9977 ± 0.0003	0.9979 ± 0.0003	0.9972 ± 0.0003	1.0019 ± 0.0003
Falstaff (1)	1.0000 ± 0.0083	**0.9910 ± 0.0005**	**0.9897 ± 0.0005**	**0.9895 ± 0.0005**	**0.9879 ± 0.0005**
SB-2½	1.0000 ± 0.0024	**1.0045 ± 0.0005**	1.0015 ± 0.0005	**0.9964 ± 0.0004**	0.9979 ± 0.0005
ORNL-11	1.0006 ± 0.0029	**1.0046 ± 0.0002**	**1.0037 ± 0.0002**	**0.9974 ± 0.0002**	0.9989 ± 0.0002
Jezebel	1.0000 ± 0.0020	1.0001 ± 0.0003	1.0002 ± 0.0003	**0.9971 ± 0.0003**	**0.9966 ± 0.0003**
Jezebel-240	1.0000 ± 0.0020	0.9996 ± 0.0003	0.9999 ± 0.0003	0.9980 ± 0.0003	1.0009 ± 0.0003
Pu Buttons (3)	1.0000 ± 0.0030	0.9988 ± 0.0003	0.9992 ± 0.0003	**0.9962 ± 0.0003**	**0.9958 ± 0.0003**
Flattop-Pu	1.0000 ± 0.0030	0.9999 ± 0.0003	1.0002 ± 0.0003	1.0016 ± 0.0003	**0.9904 ± 0.0003**
THOR	1.0000 ± 0.0006	0.9993 ± 0.0003	0.9997 ± 0.0003	**1.0057 ± 0.0003**	**1.0066 ± 0.0003**
Pu-MF-11	1.0000 ± 0.0010	1.0003 ± 0.0003	0.9998 ± 0.0003	**0.9966 ± 0.0004**	**0.9982 ± 0.0003**
HISS/HPG	1.0000 ± 0.0110	**1.0116 ± 0.0002**	**1.0114 ± 0.0002**	1.0106 ± 0.0003	**1.0134 ± 0.0003**
PNL-33	1.0024 ± 0.0021	**1.0066 ± 0.0003**	**1.0063 ± 0.0003**	1.0029 ± 0.0003	**1.0069 ± 0.0003**
PNL-2	1.0000 ± 0.0065	1.0045 ± 0.0004	1.0028 ± 0.0005	1.0031 ± 0.0005	1.0062 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ **$|\Delta k| > 2\sigma$**

Although the Criticality Validation Suite should not be used as an absolute indicator of the quality of a nuclear-data library, it can be used to provide a general indication of the likely overall performance of such a library. The results from the four libraries used in this study are compared in Table 5. Clearly, ENDF/B-VII β-1 and β-2 produce substantially better overall results than do ENDF/B-VI or JENDL-3.3. The latter two libraries produce comparable overall results, which is not surprising given that they are roughly contemporaneous.

Table 5: Summary of results.

Agreement	ENDF/B-VII β-2	ENDF/B-VII β-1	ENDF/B-VI	JENDFL-3.3
$\lvert\Delta k\rvert \leq \sigma$	18	18	13	13
$\sigma < \lvert\Delta k\rvert \leq 2\sigma$	**10**	**10**	**9**	**9**
$\lvert\Delta k\rvert > 2\sigma$	**3**	**3**	**9**	**9**

5. Some Remaining Areas of Concern

Although the results from ENDF/B-VII β-1 and β-2 are quite impressive, there are still areas where concerns remain. The cases discussed below are summarized succinctly in Table 6.

Table 6: Summary of additional cases.

Case(s)	Description
Zeus	Cylinders of HEU platters reflected by copper, moderated by graphite (intermediate spectrum) or unmoderated (fast spectrum)
Np sphere	Neptunium sphere reflected by HEU (fast spectrum)
Pu-ST-09 (3a)	Bare sphere of dilute plutonium nitrate in water (thermal spectrum)
Reflected D_2O Spheres	Spheres of uranyl fluoride in heavy water, reflected by heavy water (intermediate spectra for cases 1 and 2, thermal spectra for others)
Unreflected D_2O Cylinders	Unreflected cylinders of uranyl flouride in heavy water (thermal spectra for all cases)

5.1 ^{235}U Cross Sections in the Intermediate Resonance Region

The first four Zeus experiments were designed specifically to test the adequacy of ^{235}U cross sections in the intermediate-energy range, and the second of these benchmarks is included in the MCNP Criticality Validation Suite. As Fig. 1 shows, all four libraries produce a substantial energydependent reactivity bias over that range. Accordingly, it is recommended that the unresolved-resonance parameters for ^{235}U be reviewed before the initial release of ENDF/B-VII.

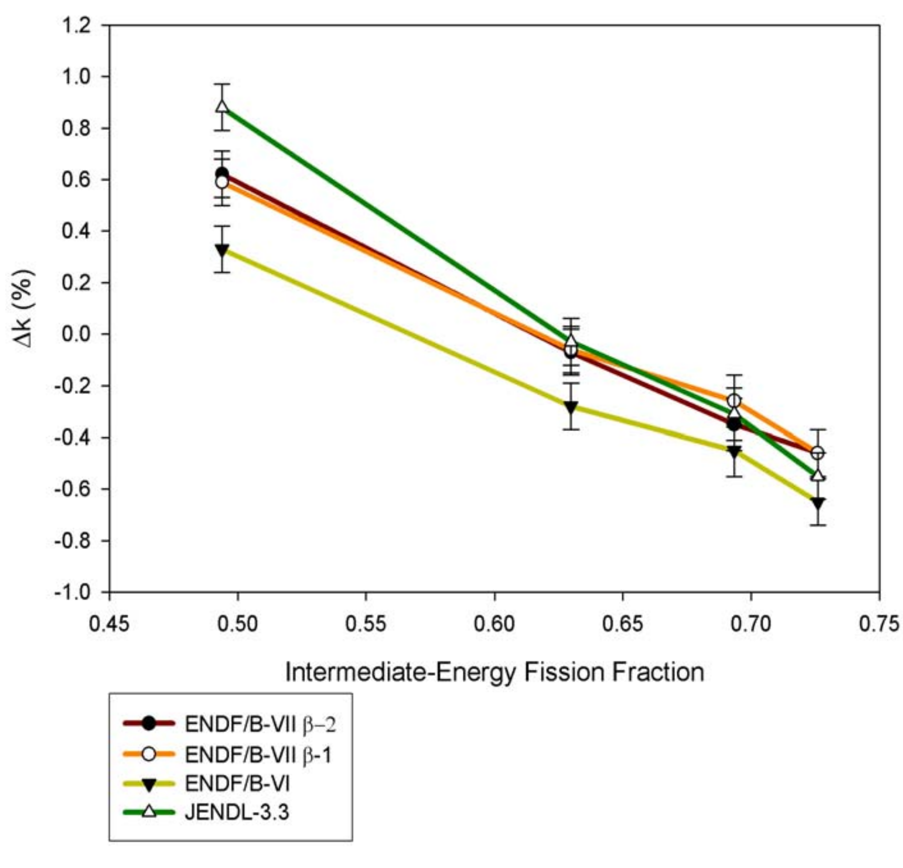
5.2 Fast Copper Cross Sections

Copper rarely plays a major role a major role in criticality benchmarks. However, the unmoderated Zeus benchmark and its predecessors are exceptions, because they use a copper reflector. As shown in Table 7, results from all four nuclear-data libraries produce values for k_{eff} that differ from the benchmark value by more than three standard deviations. When ENDF/B-V cross sections are used for copper, however, the ENDF/B-VII and JENDL-3.3 results match the benchmark value within a single standard deviation, and the ENDF/B-VI result improves as well. This pattern is not observed for the Zeus benchmarks with intermediate spectra, where replacement of the library cross sections for copper with those from ENDF/B-V has little impact on reactivity. This behavior strongly suggests that the fast cross sections for the copper isotopes should be reviewed prior to the initial release of ENDF/B-VII.

5.3 Neptunium Cross Sections

As Table 7 indicates, the agreement with the benchmark value for k_{eff} for the Np sphere improves consistently from ENDF/B-VI through ENDF/B-VII β-2. However, further improvement is needed,

Figure 1: Reactivity bias for the Zeus graphite benchmarks.



and it is recommended that the fast neptunium cross sections be reviewed further prior to the initial release of ENDF/B-VII.

5.4 Thermal Plutonium Cross Sections

Pu-ST-09 (3a) is the same size as ORNL-10 and ORNL-11, and it has a very thermal spectrum. For several years, ENDF libraries have consistently overpredicted k_{eff} for most thermal cases with plutonium, and, as Table 7 indicates, ENDF/B-VII β-2 produces the same result for this case as ENDF/B-VII β-1 and ENDF/B-VI. It is strongly recommended that the thermal cross sections for ^{239}Pu be reviewed prior to the initial release of ENDF/B-VII.

5.5 Angular Scattering Distributions for ^{2}H

Substantial changes in reactivity were observed [5] for some heavy-water solution benchmarks when the angular scattering distribution for deuterium was revised in an interim release of ENDF/B-VI. That distribution has been retained up through ENDF/B-VII β-2. However, as Table 8 shows, replacing that distribution with the one from JENDL-3.3 dramatically improves the results for the reflected spheres of heavy water. On the other hand, it causes some deterioration for the unreflected cylinders of heavy water. It is recommended that the two angular scattering distributions for ^{2}H be reviewed prior to the initial release of ENDF/B-VII in the hope that they can be reconciled.

6. Summary and Conclusions

Overall, ENDF/B-VII β-2 nuclear data produce substantial improvements relative to ENDF/B-VI for the cases in the MCNP criticality validation suite. In several cases, the improvements are quite dramatic. In particular, long-standing problems with BIG TEN, THOR, and the thermal LEU lattice benchmark have been resolved.

However, a number of areas have been identified where potential problems still remain. It is strongly recommended that as many of those areas as possible be reviewed prior to the initial release of ENDF/B-VII.

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Table 7: MCNP5 results for Other Cases.

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII β-2	ENDF/B-VII β-1	ENDF/B-VI	JENDFL-3.3
Unmoderated Zeus	1.0004± 0.0016	**1.0113 ± 0.0003** 0.9998 ± 0.0003*	**1.0116 ± 0.0003** 0.9998 ± 0.0003*	**1.0077 ± 0.0003** **0.9971 ± 0.0003***	**1.0241 ± 0.0003** 1.0000 ± 0.0003*
Np sphere	1.0019 ± 0.0036	**0.9954 ± 0.0002**	**0.9920 ± 0.0002**	**0.9889 ± 0.0003**	**0.9967 ± 0.0002**
Pu-ST-09 (3a)	1.0003 ± 0.0033	**1.0189 ± 0.0002**	**1.0189 ± 0.0002**	**1.0189 ± 0.0002**	**1.0227 ± 0.0002**

* ENDF/B-V cross sections for copper **σ < |Δk| ≤ 2σ** **|Δk| > 2σ**

Table 8: MCNP5 Results for Spheres and Cylinders of Uranyl Fluoride Reflected by Heavy Water.

Benchmark	Case	Benchmark k_{eff}	Calculated k_{eff}			
			ENDF/B-VII β-2 + JENDL-3.3 ^{2}D	ENDF/B-VII β-2	ENDF/B-VI	JENDL-3.3
Reflected D_2O Spheres	1	1.0000 ± 0.0033	0.99684 ± 0.00040	**0.98610 ± 0.00037**	**0.98387 ± 0.00041**	**0.99181 ± 0.00039**
	2	1.0000 ± 0.0036	**0.99218 ± 0.00040**	**0.98115 ± 0.00038**	**0.97982 ± 0.00041**	**0.98732 ± 0.00040**
	3	1.0000 ± 0.0039	0.99854 ± 0.00041	**0.98862 ± 0.00041**	**0.98605 ± 0.00041**	0.99790 ± 0.00044
	4	1.0000 ± 0.0046	1.00141 ± 0.00043	**0.99105 ± 0.00044**	**0.98857 ± 0.00042**	0.99711 ± 0.00044
	5	1.0000 ± 0.0052	0.99929 ± 0.00042	**0.98861 ± 0.00042**	**0.98712 ± 0.00043**	0.99561 ± 0.00044
	6	1.0000 ± 0.0059	0.99516 ± 0.00044	**0.98471 ± 0.00046**	**0.98365 ± 0.00044**	**0.99129 ± 0.00040**
Bare D_2O Cylinders	1	0.9966 ± 0.0116	1.00357 ± 0.00047	0.99161 ± 0.00049	0.99179 ± 0.00046	1.00060 ± 0.00048
	2	0.9956 ± 0.0093	**1.01033 ± 0.00050**	0.99863 ± 0.00050	0.99673 ± 0.00051	**1.00657 ± 0.00051**
	3	0.9957 ± 0.0079	**1.01855 ± 0.00052**	**1.00842 ± 0.00051**	**1.00548 ± 0.00048**	**1.01494 ± 0.00050**
	4	0.9955 ± 0.0078	**1.01609 ± 0.00052**	**1.00375 ± 0.00048**	1.00287 ± 0.00053	**1.01060 ± 0.00051**
	5	0.9959 ± 0.0077	**1.02295 ± 0.00049**	**1.01265 ± 0.00049**	**1.01139 ± 0.00052**	**1.01673 ± 0.00051**

σ < |Δk| ≤ 2σ **|Δk| > 2σ**