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Update of WIMS-D Libraries Using JENDL-3.2, ENDF/B-VI.5 and JEF-2.2

Choong-Sup Gil, Jung-Do Kim and Jongwha Chang

Korea Atomic Energy Research Institute
150 Dukjin-dong, Yusong-gu, Taejon, Korea

Abstract

The WIMS-D5 Libraries based on JENDL-3.2, ENDF/B-VI.5, and JEF-2.2 have been prepared and are being tested against the benchmark problems. Several sensitivity calculations for stability confirmation of the libraries were carried out such as the fission spectrum dependency, the self shielding effects of the elastic scattering cross sections, the self shielding effects of Pu-240 and Pu-242 capture cross sections below 4.0 eV, etc. The results of benchmark calculations with the libraries based on JENDL-3.2, ENDF/B-VI.5, JEF-2.2, and the '1986 library were intercompared. The predictions of criticalities and isotopic compositions with the updated libraries show good agreements with the measurements or the reference results. The multiplication factors with the library based on JENDL-3.2 are slightly higher than those of ENDF/B-VI.5 and JEF-2.2.

1. Introduction

The WIMS-D code¹ is one of the few reactor lattice codes that are available on a non-commercial basis. The WIMS-D/5B version has been released from the OECD/NEA Data Bank. However the available '1986 WIMS-D library² is based on old evaluated nuclear data and was empirically adjusted to achieve reasonable agreement between the calculated and measured integral parameters. As many new basic evaluated nuclear data files such as ENDF/B-VI.5, JEF-2.2, and JENDL-3.2 have been released, there are needs to create a new WIMS-D library based on the new evaluated data. The WIMS-D Library Update Project(WLUP)^{3,4} was initiated to generate a new validated WIMS-D library and was supported by the IAEA.

The WIMS-D libraries based on JENDL-3.2, ENDF/B-VI.5 and JEF-2.2 have been produced and validated by analyzing various benchmark problems. The fission spectrum is

generated from those of U-235, U-238 and Pu-239. The decay chains of fission products and actinides in the ' 1986 library were extended.

2. Sensitivity Studies

2.1 Spectrum Dependency

A single fission spectrum is allowed in the WIMS-D library. There are needs to check the influence of different spectra. The spectral indices were calculated with the library based on JENDL-3.2 for the sensitivity tests of the spectra in the TRX-1 and BAPL-1 lattices⁵. The integral parameters are defined as following.

ρ^{28} : The ratio of epithermal to thermal capture reaction rates in U-238,

ρ^{25} : The ratio of epithermal to thermal fission reaction rates in U-235,

δ^{28} : The ratio of the total fission reaction rates of U-238 and U-235,

C^* : The ratio of the capture reaction rates in U-238 to the fission reaction rates in U-235.

The reference values in Table-1a, -1b were calculated with the library of JENDL-3.2 of which spectrum was weighted by the U-235(57%), U-238(8%) and Pu-239(35%). The compared values(spectrum) were calculated with the spectrum which was generated from the ratios of U-235 and U-238 of the lattices. The calculated integral values in Table-1a, -1b were not sensitive to the spectra except for the δ^{28} quantity.

Table-1a. The Calculated Spectral Indices in the TRX-1 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}	C^*
Reference	1.179023	0.99269	1.3574	0.0974	0.0969	0.8015
Spectrum	1.177222	0.99250	1.3580	0.0974	0.0944	0.8018

Table-1b. The Calculated Spectral Indices in the BALP-1 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}
Reference	1.14420	0.99915	1.4106	0.0823	0.0753
Spectrum	1.14290	0.99912	1.4109	0.0822	0.0734

2.2 Self Shielding Effects of Elastic Scattering Cross Sections

The effects with fully shielded and infinite diluted elastic scattering cross sections were calculated in the TRX-1, BAPL-1 and TCA lattices⁶. The WIMS-D code can not consider a self shielding effect of elastic scattering cross section. The first row in Table-2a is the results with the library based on JENDL-3.2 in which the elastic cross sections were generated at appropriate background cross sections. The second row is the results with the library generated at the accurate background cross sections of the considered lattices. The third one is the results with the library of which all cross sections except elastic scattering were infinitely diluted. The last one is the results with all cross sections infinitely diluted. The reference results show good agreements with those of the accurate library(second row). The differences between the third and last one are caused by self shielding of the elastic scattering cross section. The maximum differences from the self shielding of elastic scattering in k-eff show about 1% in the lattices. The ρ^{28} values in the TRX-1 show a difference of 2%.

Table 2-a. The Self Shielding Effects of Elastic Scattering Cross Sections in the TRX-1 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}	C*
Reference at σ_0 (=800b, U-235) (=28b, U-238)	1.179023	0.99269	1.3574	0.0974	0.0969	0.8015
All C.S. at σ_0 (=2600b, U-235) (=28b, U-238)	1.179050	0.99271	1.3575	0.0975	0.0969	0.8014
Inf. Dil. (fully shielded elastic)	1.178144	0.99148	1.3638	0.0976	0.0971	0.8035
All Inf. Dil.	1.181688	1.00087	1.3356	0.0960	0.0960	0.7951

Table 2-b. The Self Shielding Effects of Elastic Scattering Cross Sections in the BAPL-1 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}
Reference at σ_0 (=800b, U-235) (=28b, U-238)	1.14420	0.99915	1.4106	0.0823	0.0753
All C.S. at σ_0 (=5000b, U-235) (=64b, U-238)	1.14395	0.99925	1.4124	0.0824	0.0753
Inf. Dil. (fully shielded elastic)	1.14353	0.99828	1.4156	0.0825	0.0754
All Inf. Dil.	1.14486	1.00414	1.4037	0.0819	0.0749

Table 2-c. The Self Shielding Effects of Elastic Scattering Cross Sections in the TCA-PuO₂-UO₂ Lattices

Lattices	Library	k-inf.	k-eff.
2.42Pu	Reference at σ_0 (=2,000b, Pu-240) (=50,000b, Pu-242)	1.35025	0.99761
	All cross sections at σ_0 (=20,000b, Pu-240) (=200,000b, Pu-242)	1.34666	0.99505
	Inf. Dil. (fully shielded elastic)	1.34574	0.99412
	All Inf. Dil.	1.34615	1.00017
5.55Pu	Reference at σ_0 (=2,000b, Pu-240) (=50,000b, Pu-242)	1.24717	1.00667
	All cross sections at σ_0 (=20,000b, Pu-240) (=200,000b, Pu-242)	1.24640	1.00607
	Inf. Dil. (fully shielded elastic)	1.24624	1.00587
	All Inf. Dil.	1.24640	1.00080

2.3 Influence of Pu-240 and Pu-242 capture resonances below 4 eV

The WIMSD code is not allowed to handle the resonance self shielding below 4 eV. However there are some nuclides including the resonances below the energy. Especially the large capture resonances of Pu-240 and Pu-242 at 1 eV and 2.67 eV, respectively, are important. The energy group structure of WIMSD code is very fine around 1 eV. So the resonance effect of Pu-240 at 1.0 eV can be mitigated. As the energy group structure at 2.67 eV is relatively coarse, the resonance of Pu-242 should be considered appropriately. The newly generated library includes two nuclides for Pu-242 at 50,000(ID=1242, L) and 1,000(ID=242, H) barns of background cross sections, respectively. Table 3 shows the comparison of the results with different libraries. Because the background cross sections of the TCA lattices are very large(refer to Table 2-c), it seems reasonable to use the data of Pu-242(ID=1242,L).

Table 3. Comparison of the Results with the Libraries and Pu-242 Data in the TCA PuO₂-UO₂ Lattices

Lattices	Libraries	k-inf.		k-eff.	
		Pu-242L (1242)	Pu-242H (242)	Pu-242L (1242)	Pu-242H (242)
2.42Pu	JENDL-3.2	1.35025	1.34833	0.99761	0.99623
	WIMS 1986	1.34047	1.34047	0.98516	0.98516
	ENDF/B-VI.5	1.34663	1.34416	0.99331	0.99154
	JEF-2.2	1.34744	1.34530	0.99496	0.99343
2.98Pu	JENDL-3.2	1.34552	1.34393	1.00151	1.00037
	WIMS 1986	1.33511	1.33511	0.98851	0.98851
	ENDF/B-VI.5	1.34196	1.33992	0.99739	0.99592
	JEF-2.2	1.34246	1.34068	0.99862	0.99735
4.24Pu	JENDL-3.2	1.30588	1.30478	1.00495	1.00412
	WIMS 1986	1.29500	1.29500	0.99141	0.99141
	ENDF/B-VI.5	1.30246	1.30104	1.00115	1.00006
	JEF-2.2	1.30243	1.30123	1.00168	1.00075
5.55Pu	JENDL-3.2	1.24717	1.24798	1.00667	1.00731
	WIMS 1986	1.23711	1.23711	0.99387	0.99387
	ENDF/B-VI.5	1.24368	1.24472	1.00295	1.00378
	JEF-2.2	1.24338	1.24429	1.00307	1.00379

2.4 PURR and UNRESR Module Effects of NJOY

The unresolved resonance cross sections of the ENDF data can be processed using the UNRESR or PURR module of the NJOY code⁷. The self shielding factors calculated with the UNRESR module for some nuclides are slightly larger than 1.0. These are not physically reasonable. The PURR module of the NJOY is not stable yet. The results with UNRESR and PURR module were compared in table 4. It is general that the threshold energies of unresolved resonances are relatively high comparing with the sensitive energies in the light water reactors. The differences of the results with the UNRESR and PURR modules are negligible in analyzing the light water reactors.

Table 4-a. Comparison of the Results with UNRESR and PURR of the NJOY in the TRX-1 Lattices

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}	C*
UNRESR	1.179023	0.99269	1.3574	0.0974	0.0969	0.8015
PURR	1.179085	0.99270	1.3570	0.0974	0.0969	0.8014

Table 4-b. Comparison of the Results with UNRESR and PURR of the NJOY in the BAPL-1 Lattices

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}
UNRESR	1.14420	0.99915	1.4106	0.0823	0.0753
PURR	1.14426	0.99917	1.4102	0.0823	0.0753

4. Benchmark Lattices

The validations of the libraries were performed through the analyses of various benchmark lattices. The benchmarks for the LWRs are the TRX-, BAPL-series, DIMP-1A, TCA, and NEA plutonium recycling lattices. The benchmark lattices are briefly described as following.

- (a) TRX-1, -2(1.3% enriched U-metal fueled, H₂O moderated),
BAPL-1, -2, -3(1.3% enriched UO₂ fueled, H₂O moderated),
DIMP-1A(3% enriched UO₂ fueled, H₂O moderated) critical lattices⁸.
- (b) Tank Type Critical Assembly(TCA)
 - Uranium(2.6w% enriched UO₂ fueled, H₂O moderated),
 - MOX(3.0w% enriched Pu-UO₂ fueled, H₂O moderated) critical lattices
- (c) OECD/NEA Pu Recycling Lattices⁹
 - NEA-A($V_m/V_f = 1.9284$, Pu total = 12.5w%, Pu fissile = 6w% :
(Pu238:Pu239:Pu240:Pu241:Pu242 = 4:36:28:12:20)
 - NEA-B($V_m/V_f = 1.9284$, Pu total = 4.0w%, Pu fissile = 2.8w% :
(Pu238:Pu239:Pu240:Pu241:Pu242 = 1.8:59:23:12.2:4)

5. Results and Discussions

Several sensitivity calculations were performed for the library stability. A single fission spectrum is only available in the WIMS-D library. The integral parameters were not sensitive to the fission spectrum of the library. The self shielding effects of elastic scattering cross sections can affect on the integral parameters. Appropriate self shielded elastic scattering cross sections of the library should be generated. The cross sections of the nuclides having resonances below 4 eV should be carefully generated.

The criticality predictions with the different libraries were performed and compared with the measured values in Table 5 ~ 11. The keffective values with all libraries are slightly underpredicted. The k-effective values with JENDL-3.2 are the highest, the JEF-2.2 are in the middle, and those of the ENDF/B-VI are the lowest. The spectral indices in the lattices agree with the measured quantities within the uncertainties of the experiments. Table 12 and 13 show the comparison of isotopic composition in the OECD/NEA burnup credit and plutonium recycling benchmarks. The calculated quantity of Sm-149 with the new libraries shows more than 30 % from the measurements in Table 12. The measured values of Sm-149 are questionable. The calculated amounts of Pu-238 and Sm-152 show relatively large differences from the measurements. In Table 13, the amounts of Cm-242 and Cm-243 are overpredicted more than 2

times, compared with the reference values. The calculated value of Pu-238 shows a difference from the reference out of uncertainty.

6. Conclusions

The WIMS-D/5B libraries based on new evaluated data have been generated and are being tested through analyses of the benchmark lattices. The libraries are not adjusted to the measured integral parameters. The new libraries show stabilities in fission spectrum, self shielding of elastic scattering cross sections. The results with the libraries show good agreements with the measurements. The multiplication factors with JENDL-3.2 are slightly higher than those of JEF-2.2 and ENDF/B-VI.5. A best library, which will be generated from the selections of the best nuclide data from ENDF/B-VI, JENDL-3.2 and JEF-2.2 will be recommended at the end of 2001.

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Table 5. Comparison of C/E Integral Parameters in the TRX-1 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}	C*
Exp. (% Err.)		1.00000 (0.3)	1.320 (1.6)	0.0987 (1.0)	0.0946 (4.3)	0.797 (1.0)
JENDL-3.2	1.179023*	0.99269+	1.028	0.987	1.024	1.006
WIMS1986	1.18686	0.99313	1.016	0.992	1.067	0.990
ENDF/B-VI.5	1.17569	0.98777	1.029	0.990	1.053	1.010
JEF-2.2	1.17842	0.99168	1.026	0.995	1.037	1.009

* Calculated Value

+ Calculated/Experimental Value

Table 6. Comparison of C/E Integral Parameters in the TRX-2 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}	C*
Exp. (% Err.)		1.00000 (0.1)	0.837 (1.9)	0.0614 (1.3)	0.0693 (5.1)	0.647 (0.93)
JENDL-3.2	1.16525	0.99447	1.016	0.976	0.997	0.999
WIMS1986	1.17142	0.99482	1.004	0.980	1.040	0.986
ENDF/B-VI.5	1.16195	0.99009	1.016	0.977	1.019	1.002
JEF-2.2	1.16346	0.99238	1.014	0.982	1.007	1.002

Table 7. Comparison of C/E Integral Parameters in the BAPL-1 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}
Exp. (%Err.)		1.00000 (0.10)	1.390 (0.72)	0.0840 (2.4)	0.0780 (5.1)
JENDL-3.2	1.14420	0.99915	1.015	0.980	0.965
WIMS1986	1.14873	0.99887	1.010	0.985	1.008
ENDF/B-VI.5	1.13919	0.99377	1.016	0.980	0.983
JEF-2.2	1.14228	0.99755	1.013	0.985	0.974

Table 8. Comparison of C/E Integral Parameters in the BAPL-2 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}
Exp. (%Err.)		1.00000 (0.1)	1.120 (0.89)	0.0680 (1.5)	0.0700 (5.7)
JENDL-3.2	1.14850	0.99898	1.048	0.988	0.927
WIMS1986	1.15247	0.99820	1.043	0.994	0.969
ENDF/B-VI.5	1.14374	0.99390	1.049	0.987	0.941
JEF-2.2	1.14638	0.99712	1.046	0.993	0.934

Table 9. Comparison of C/E Integral Parameters in the BAPL-3 Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	ρ^{25}	δ^{28}
Exp. (%Err.)		1.00000 (0.1)	0.906 (1.1)	0.0520 (1.9)	0.0570 (5.3)
JENDL-3.2	1.13463	0.99953	1.017	0.994	0.935
WIMS1986	1.13797	0.99868	1.013	1.002	0.977
ENDF/B-VI.5	1.13023	0.99490	1.018	0.992	0.947
JEF-2.2	1.13224	0.99734	1.015	0.998	0.940

Table 10. Comparison of C/E Integral Parameters in the DIMP-1A Lattice

Quantities	k-inf.	k-eff.	δ^{28}	C*
Exp. (%Err.)		1.00000 (0.1)	0.0962 (3.3)	0.647 (0.46)
JENDL-3.2	1.26434	1.00041	0.893	1.006
WIMS1986	1.26654	0.99393	0.933	0.996
ENDF/B-VI.5	1.25603	0.99195	0.918	1.012
JEF-2.2	1.26081	0.99792	0.901	1.009

Table 11. Comparison of k-inf. and k-eff. Values the TCA UO₂ Lattices

Lattices		k-inf.	k-eff.
1.50U	JENDL-3.2	1.36345	0.99848
	WIMS 1986	1.36634	0.99212
	ENDF/B-VI.5	1.35619	0.99090
	JEF-2.2	1.36101	0.99686
1.83U	JENDL-3.2	1.37551	1.00034
	WIMS 1986	1.37820	0.99407
	ENDF/B-VI.5	1.36868	0.99322
	JEF-2.2	1.37287	0.99844
2.48U	JENDL-3.2	1.37278	0.99827
	WIMS 1986	1.37530	0.99244
	ENDF/B-VI.5	1.36660	0.99185
	JEF-2.2	1.36985	0.99596
3.00U	JENDL-3.2	1.35695	1.00110
	WIMS 1986	1.35945	0.99575
	ENDF/B-VI.5	1.35115	0.99509
	JEF-2.2	1.35383	0.99852

Table 12. Comparison of Isotopic Composition in OECD/NEA Burnup Credit

Calculational Criticality Benchmark Phase 1B (Burnup = 27.35 GWD/TU)

Isotopes	JENDL-3.2	1986 Lib.	ENDF/B-VI.5	JEF-2.2
U -234	0.2*	-2.5	-1.1	-1.0
U -235	-2.9	-3.7	-1.8	-1.6
U -236	-0.3	0.7	2.5	-0.4
U -238	-0.6	-0.6	-0.6	-0.6
Pu-238	-14.3	-36.4	-11.5	-9.6
Pu-239	-3.0	-3.5	-2.9	-2.8
Pu-240	-1.6	1.4	-2.8	-2.2
Pu-241	-2.8	-4.4	-3.4	-5.0
Pu-242	-4.2	-9.6	-7.8	-8.3
Am-241	0.0	0.0	0.0	0.0
Am-243	0.0	0.0	0.0	0.0
Np-237	2.5	-4.1	-2.0	-1.1
Mo- 95	0.0	0.0	0.0	0.0
Tc- 99	0.0	0.0	0.0	0.0
Ru-101	0.0	0.0	0.0	0.0
Rh-103	0.0	0.0	0.0	0.0
Ag-109	0.0	0.0	0.0	0.0
Cs-133	0.3	-0.5	-0.1	-2.3
Cs-135	4.5	3.4	4.5	3.2
Nd-143	-0.3	3.0	-0.8	-0.3
Nd-145	0.2	-1.2	-0.7	0.1
Sm-147	0.0	0.0	0.0	0.0
Sm-149	-36.4	-19.4	-35.8	-36.4
Sm-150	-9.1	-3.3	-8.4	-8.6
Sm-151	0.0	0.0	0.0	0.0
Sm-152	12.7	12.2	8.0	8.4
Eu-153	-1.4	-13.6	-1.3	0.5
Gd-155	0.0	0.0	0.0	0.0
Gd-157	0.0	0.0	0.0	0.0
O - 16	0.0	0.0	0.0	0.0

* Difference from the measurement(%)

Table 13. Comparison of Isotopic Composition in Physics of Plutonium Recycling

Benchmark A – Highly Degrade Plutonium (Burnup = 50.0 GWD/TU)

Isotopes	Reference	JENDL-3.2	ENDF/B-VI.5	JEF-2.2
U -234	3.0*	6.8 ⁺	8.1	8.7
U -235	1.0	2.2	2.8	3.4
U -236	3.2	-4.8	-0.1	-6.1
U -238	0.1	0.0	0.1	0.1
Np-237	9.5	5.9	-0.1	-2.0
Pu-238	4.7	16.6	22.1	22.8
Pu-239	1.2	1.8	3.0	2.7
Pu-240	3.2	-3.5	-2.2	-1.7
Pu-241	3.4	4.0	3.4	2.5
Pu-242	8.2	4.2	3.6	3.6
Am-241	3.9	6.0	5.1	1.8
Am-242m	16.9	8.8	1.7	4.7
Am-243	25.6	-16.5	-15.8	-17.5
Cm-242	5.3	104.1	143.1	136.5
Cm-243	7.3	95.5	115.2	130.9
Cm-244	3.8	-1.1	-1.8	-3.7
Mo- 95	8.0	5.1	1.7	3.0
Tc- 99	5.9	2.3	-0.7	0.1
Ru-101	2.1	-1.6	-1.1	0.7
Rh-103	4.5	-1.6	0.9	-1.4
Pd-105	2.5	-1.9	-0.3	1.0
Pd-107	1.4	0.6	-3.8	-4.9
Pd-108	3.3	0.9	-2.9	-2.3
Ag-109	18.7	22.1	12.7	6.7
Xe-131	6.9	-0.3	-2.3	2.0
Xe-135	2.8	4.4	3.5	0.0
Cs-133	5.3	3.3	2.5	0.1
Cs-135	1.7	2.1	1.0	-2.2
Nd-143	13.7	-5.3	-7.6	-6.7
Nd-145	5.7	-1.2	-4.3	-2.9
Pm-147	29.3	8.6	7.5	8.6
Pm-148m	12.6	12.0	6.5	8.7
Sm-149	18.6	-7.9	-6.6	-7.9
Sm-150	7.3	-5.3	-7.1	-5.6
Sm-151	31.4	-6.7	-8.1	-7.2
Sm-152	15.8	5.5	-2.2	-0.7
Eu-153	11.5	8.4	5.0	8.4
Eu-154	16.8	-5.9	-2.4	2.3
Eu-155	40.2	-24.6	-47.6	37.3
O – 16	0.0	0.0	0.0	0.0

* Reference uncertainty(%)

⁺ Difference from the reference value(%)