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Benchmark Test and Adjustment of an Updated Library from ENDF/B-IV

Jung-Do Kim and Jong Tai Lee

Korea Advanced Energy Research Institute
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ENDF/B-IV로 생산된 열중성자로용 라이브러리의 벤치마크 계산 및 수정

김 정 도 · 이 종 태

한국에너지연구소
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Abstract

A LEOPARD library was updated from the ENDF/B-IV evaluated data using ETOT-3—ETOG-3 code system. The applicability of the library was assessed through benchmark tests for many light water-moderated critical assemblies, and adjustment techniques were applied to group constants to fit critical experiments. It is confirmed that the library from ENDF/B-IV, coupled with the use of LEOPARD code, leads to reasonable results for light water-moderated UO_2 fueled cores with the above adjustments.

요 약

ETOT-3—ETOG-3 전산체계와 ENDF/B-IV 평가핵자료를 이용하여 LEOPARD코드용 핵자료 라이브러리를 생산하였다. 그리고 생산된 라이브러리의 신뢰성을 입증하기 위하여, 선정된 많은 실험자료에 대한 임계계산을 수행하였다. 이 결과를 토대로 경수형 UO_2 핵연료계에 대한 수정, 평가계산을 수행하여 조정된 라이브러리가 유용함을 확인하였다.

1. Introduction

The LEOPARD[1] code developed by the Westinghouse Co. may be regarded as one of the basic physics codes for light water-moderated reactors.

This code has been frequently applied to calculations of few group constants, the neutron multiplication factor or fuel depletion effects for PWR core analysis.

The extensive developement of nuclear

power calls for a highly accurate knowledge of nuclear constants of fissile and structural materials of the core.

One of the principal advantages of the LEOPARD is to have its own built-in data library, but the library is relatively old and recent nuclear data evaluations are not taken into account. In addition, LEOP ARD library does not contain enough nuclides to be desirable or necessary for PWR core analysis. Consequently, there has arisen a need to update these library from recent and more accurate evaluated nuclear data.

The data in the LEOPARD library with 172+54 group structures was generated from ENDF/B-IV evaluated data using the ETOT-3—ETOG-3 processing code system.

And then, an applicability of the updated library was assessed through benchmark tests for many light water-moderated critical assemblies. Adjustment techniques were also applied to group constants to fit with the results obtained from critical experiments.

2. Update of LEOPARD Library

2.1. Description of Old Library

The built-in library data in the released LEOPARD were original MUFT[2] and SOF OCATE library[3] data. The MUFT library was mainly based on tape 0 in report WAPD-TM-224 (1960), while the SOFOCA TE library was based on report WAPD-TM-67 (1957) with subsequent modifications.

Therefore, almost all the original LEOP ARD library data were those in the 1950s, and raw data unavailable were replaced by those of similar nuclide. For instance, thermal transport cross sections of U-233, U-236, U-238, and those of Pu-239 and Pu-241 were taken to be 9.972 barns and 10.9692 barns, respectively.

In fast regions, all elastic scatterings of Pu-240, Pu-241 and Pu-242 were replaced by those of U-235. And all inelastic scatterings of Pu-240, Pu-241 and Pu-242 were also replaced by those of Pu-239.

In addition, some of bias factors to compensate the differences between calculated mean k_{eff} and experimental values were considered in this library. Namely, the bias factor of 1.0036[4] was applied to the LEOPARD calculation by uniformly adjusting ν values(neutrons per fission) of all fissile nuclides. Especially the bias factor of U-235 in fast groups was 0.9914.

2.2. Procedure of Library Generation

The ETOT-3[5]—ETOG-3[6] system has been established to process data from ENDF/B-IV to TEMPEST[7] and MUFT[8] format.

The ETOT-3 code was used to generate thermal cross sections of TEMPEST 246 group format and the ETOG-3 code fast data of MUFT 54 group format.

In ETOT-3 calculations, fine group cross sections were not group averaged values but point values. In calculations of the resolved resonance region, single or multi-level Breit-Wigner formula was used to calculate microscopic cross sections.

In ETOG-3 calculations, group data were generated using a "1/E + U-235 fission spectrum" weighting function. The fission spectrum joined 1/E at 67.4 keV(lower boundary of 20th group). Similarly, single of multi-level Breit-Wigner parameters were used to generate resonance data.

54 group fission spectra of U-235 and Pu-239 were also generated as sources in MUFT calculation, respectively.

Thermal 246 group data and fast 54 group data obtained from ETOT-3—ETOG-3 system can not be directly used as a LEO PARD input. Since the LEOPARD uses very large blocks of library data, a separate library-producing precursor code, SPO TS, has been provided to make up the library.

In this updating procedure, the SPOTS4[9] code (an extension of the SPOTS) was used in the library generation.

As the result, an updated ENDF/B-IV LEOPARD library was prepared for all materials available at present in the code and other nuclides which may be considered to be disirable additions.

3. Benchmark Test

In order to estimate the applicability of the updated library for the design analysis of light water-moderated reactor, benchmark calculations have been performed for 59 critical experiments.

There are at least two approaches that one can take to determine the adequacy of cross section data for reactor. The first approach involves detailed calculations for a few critical experiments. Comparison between experiments and calculations are made for such parameter as the multiplication factor, thermal flux disadvantage factor, various cadmium ratios and quantities pertinent to the fast fission and resonance absorption effects. If adequate agreement is found for all this parameters, it is assumed that all important reaction rates are being calculated satisfactorily and cross section data used in the calculation are adequate.

The second approach is to calculate a single parameter such as the multiplication factor for a large number of experiments which include a wide range of variables. Although errors in several reaction rates could cancel to give adequate agreement in k_{eff} for some cases, it is extremely unlikely that the errors would cancel over a wide range of variables. Consequently if the agreement in k_{eff} is good, it can be assumed that the important reaction rates are being calculated properly.

This second apprach has been adopted in this paper to check the adequacy of the updated library.

Fig. 1 shows the flow diagram for production and benchmark test of LEOPARD library from ENDF/B-IV.

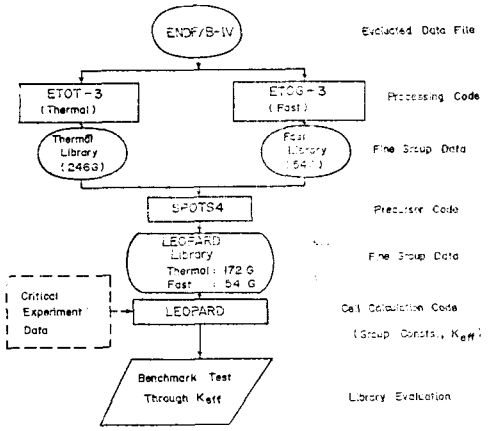

Fig. 1. Flow Diagram for Production and Benchmark Test of LEOPARD Library from ENDF/B-IV

3.1. Description of Critical Assemblies

Experimental data for a large number of critical assemblies using UO_2 and PuO_2-UO_2 fuels have been collected from available literatures.[10)~20)] Most of the cases were limited to assemblies for which experimental bucklings have been reported.

Using the experimental buckling to represent leakage, the effective multiplica-

Table 1. Data for UO_2 Critical Experiments

Case No.	Enrich. at.%	H_2O:U Vol. Ratio	Fuel Den. g/cm³	Pellet Dia. cm	Clad Mat.	Clad O. D. cm	Clad Thick. cm	Latt. Pitch cm	B-10 Conc. ppm	Crit. Buck. m^{-2}	Reference
1	2.734	2.18	10.18	.7620	SS 304	.8954	.04085	1.0287	0	40.75	10
2	2.734	2.93	10.18	.7620	SS 304	.8954	.04085	1.1049	0	53.23	10
3	2.734	3.86	10.18	.7620	SS 344	.8954	.04085	1.1938	0	63.26	10
4	2.734	7.02	10.18	.7620	SS 304	.8954	.04085	1.4554	0	65.64	11
5	2.734	8.49	10.18	.7620	SS 304	.8954	.04085	1.5621	0	60.07	11
6	2.734	10.38	10.18	.7620	SS 304	.8954	.04085	1.6891	0	52.92	11
7	2.734	2.50	10.18	.7620	SS 304	.8954	.04085	1.0617	0	47.50	12
8	2.734	4.51	10.18	.7620	SS 304	.8954	.04085	1.2522	0	68.80	12
9	3.745	2.50	10.37	.7544	SS 304	.8600	.04060	1.0617	0	68.30	12
10	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	0	95.10	12
11	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	0	95.68+	13
12	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	456	74.64+	13
13	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	709	63.66+	13
14	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	1260	40.99+	13
15	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	1334	38.39+	13
16	3.745	4.51	10.37	.7544	SS 304	.8600	.04060	1.2522	1477	33.38+	13
17	5.809	3.13	10.19	.9068	SS 304	.9931	.03810	1.3208	0	117.60	14
18	4.069	2.55	9.46	1.1278	SS 304	1.2090	.04060	1.5113	0	88.00	15
19	4.069	2.55	9.46	1.1278	SS 304	1.2090	.04060	1.5113	3392	17.20	15
20	4.069	2.14	9.46	1.1278	SS 304	1.2090	.04060	1.4500	0	79.00	15
21	3.037	2.64	9.28	1.1268	SS 304	1.2701	.07163	1.5550	0	50.75	16
22	3.037	8.16	9.28	1.1268	SS 304	1.2701	.07163	2.1980	0	68.81	16
23	4.069	2.59	9.45	1.1268	SS 304	1.2701	.07163	1.5550	0	69.25	16
24	4.069	3.53	9.45	1.1268	SS 304	1.2701	.07163	1.6840	0	85.52	16
25	4.069	8.02	9.45	1.1268	SS 304	1.2701	.07163	2.1980	0	92.84	16
26	4.069	9.90	9.45	1.1268	SS 304	1.2701	.07163	2.3810	0	91.79	16
27	1.328	3.02	7.53	1.5265	Al	1.6916	.07110	2.2050*	0	28.37	17
28	1.328	3.95	7.53	1.5265	Al	1.6916	.07110	2.3590*	0	30.17	17
29	1.328	4.95	7.53	1.5265	Al	1.6916	.07110	2.5120*	0	29.06	17
30	1.328	3.93	7.52	.9855	Al	1.1506	.07110	1.5580*	0	25.28	17
31	1.328	4.89	7.52	.9855	Al	1.1506	.07110	1.6520*	0	25.21	17
32	1.328	2.88	10.53	.9728	Al	1.1506	.07110	1.5580*	0	32.59	17
33	1.328	3.58	10.53	.9728	Al	1.1506	.07110	1.6520*	0	35.47	17
34	1.328	4.83	10.53	.9728	Al	1.1506	.07110	1.8060*	0	34.22	17
35	2.490	2.84	10.24	1.0297	Al	1.2060	.08130	1.5113	1675	20.20	15
36	2.096	2.06	10.38	1.5240	Al	1.6916	.07112	2.1737	0	58.00	18
37	2.096	2.06	10.38	1.5240	Al	1.6916	.07112	2.4052	0	80.60	18
38	2.096	4.12	10.38	1.5240	Al	1.6916	.07112	2.6162	0	85.70	18
39	2.096	6.14	10.38	1.5240	Al	1.6916	.07112	2.9891	0	77.00	18
40	2.096	8.20	10.38	1.5240	Al	1.6916	.07112	3.3255	0	61.60	18
41	2.628	1.50	10.40	1.2500	Al	1.4170	.07600	1.8490	0	83.30+	19
42	2.628	1.83	10.40	1.2500	Al	1.4170	.07600	1.9560	0	94.30+	19
43	2.628	2.48	10.40	1.2500	Al	1.4170	.07600	2.1500	0	98.30+	19
44	2.628	3.00	10.40	1.2500	Al	1.4170	.07600	2.2930	0	95.20+	19

* Hexagonal Lattice : All others are square.

+ These bucklings were not measured directly but were inferred from critical loadings.

tion factor can be calculated in a "point model", without performing any diffusion calculations.

Of the 59 assemblies studied, 44 cases are UO_2 cores and 15 cases PuO_2-UO_2.

U-235 enrichments of UO_2 fuels vary from 1.328 to 5.809 %; moderator-to-fuel volume ratios(H_2O : U) vary from approximately 2.06 to 18.37. Pellet diameters from 0.7544 to 1.5265 cm are used; both stainless steel and aluminum clad for UO_2 fuels and zircalloy-2 clad for PuO_2-UO_2 fuels are studied as much as both square and hexagonal lattice arrays.

The data for all the collected assemblies are given in Table 1 and Table 2, seperately for UO_2 and PuO_2-UO_2 fuels.

As shown in the above Tables, it is felt that the wide variation in parameters provides a severe test for the updated cross section library.

Table 2. Data for PuO_2-UO_2 Critical Experiments

Case No.	PuO_2/ Pu-240 w/o	H_2O:F Vol. Ratio	Fuel Den. g/cm³	Pellet Dia. cm	Clad Mat.	Clad O. D. cm	Clad Thick. cm	Latt. pitch cm	B-10 Conc. ppm	Crit. Buck. m^{-2}	Reference
45	2.0/ 7.65	2.51	9.54	1.283	Zr-2	1.443	0.076	1.753	0	69.1	20
46	2.0/ 7.65	18.37	9.54	1.283	Zr-2	1.443	0.076	3.505	0	50.3	20
47	2.0/ 7.65	9.70	9.54	1.283	Zr-2	1.443	0.076	2.694	0	98.4	20
48	2.0/ 7.65	7.76	9.54	1.283	Zr-2	1.443	0.076	2.479	0	105.9	20
49	2.0/ 7.65	7.76	9.54	1.283	Zr-2	1.443	0.076	2.479	261	83.7	20
50	2.0/ 7.65	7.76	9.54	1.283	Zr-2	1.443	0.076	2.479	526	63.1	20
51	2.0/ 7.65	2.48	9.54	1.283	Zr-2	1.443	0.076	1.753	526	58.3	20
52	2.0/ 7.65	2.48	9.54	1.283	Zr-2	1.443	0.076	1.753	261	62.6	20
53	2.0/ 7.65	3.43	9.54	1.283	Zr-2	1.443	0.076	1.905	0	90.0	20
54	2.0/23.5	7.80	9.54	1.283	Zr-2	1.443	0.076	2.479	0	79.5	20
55	2.0/23.5	9.72	9.54	1.283	Zr-2	1.443	0.076	2.694	0	73.3	20
56	3.01/22.02	2.42	6.056	1.065	Zr-2	1.223	0.070	1.825	0	80.8+	19
57	3.01/22.02	2.98	6.056	1.065	Zr-2	1.223	0.070	1.956	0	82.8+	19
58	3.01/22.02	4.24	6.056	1.065	Zr-2	1.223	0.070	2.225	0	77.9+	19
59	3.01/22.02	5.55	6.056	1.065	Zr-2	1.223	0.070	2.474	0	65.1+	19

+ These bucklings were not measured directly but were inferred from critical loadings.

3.2. Criticality Calculation

For all cases, effective multiplication factors were calculated using experimental buckling, geometry and compositions in Table 1 & 2 by the LEOPARD code with the updated library. The results are given in the form of the ratio of calculated to experimental value(C/E) for each critical assembly.

3.3. Result and Discussion

Results of k_{eff} calculations for 59 critical assemblies are given in Table 3 and Table 4. To extract the characteristics of the library data, the statistical average, the standard deviation and the average of absolute difference from unity were analysed. These are also shown in the above Tables. In k_{eff} calculations for mixed-oxide (PuO_2-UO_2) cores, fission spectrum of U-235 or Pu-239 was used as source data.

From Table 3 of 44 UO_2 cases, statistical values give the average k_{eff} of 0.9954, the standard deviation of 1.52 % and the average deviation from unity of 0.0123.

This result shows the updated library data underpridict k_{eff} by~0.5 % for UO_2 cores. And the standard deviation of 1.52 %

Table 3. Comparison of Calculated Values of K_{eff} of Experimental UO_2 Critical Assemblies

Case Number	K_{eff}	Case Number	K_{eff}
1	0.97616	23	0.99140
2	0.98980	24	0.99570
3	0.99608	25	1.01099
4	1.00764	26	0.99464
5	1.00949	27	0.98997
6	1.00443	28	0.99622
7	0.98077	29	0.99605
8	0.99350	30	0.98875
9	0.98757	31	0.99201
10	1.00424	32	0.98872
11	1.00327	33	0.99608
12	0.99601	34	0.99595
13	0.99283	35	0.99229
14	0.98860	36	1.05236
15	0.98741	37	1.00991
16	0.98543	38	0.99327
17	1.00410	39	0.97454
18	0.98961	40	0.95412
19	0.98401	41	1.01933
20	0.97781	42	1.01055
21	0.98008	43	1014.63
22	0.98212	44	1.01839

Average K_{eff}	: 0.99539
Standard Deviation	: 0.01517
Average $\|K_{eff}-1.0\|$	: 0.01232
Without Case No. 36 through 44	
Average K_{eff}	: 0.99285
Standard Deviation	: 0.00862
Average $\|K_{eff}-1.0\|$	: 0.00968

or the average deviation from unity of 0.0123 shows that calculated data are scattered.

In general, Aerojet General Corporation (AGC) and JAERI data (Table 1) give a large discrepancy from unity. In referennce 13, experimental buckling uncertainties of AGC measurements are larger than normal. And critical bucklings of JAERI data were inferred from critical loadings. In addition to buckling uncertainties, other effects that increase the standard deviation of the calculated results include impurities in the fuel, clad and moderator (impurities were neglected in the calculations) and uncertainties in physical parameters such as dimensions, densities and enrichments. Actually, disregarding cases 36 through 44 gives the standard deviation of 0.86%.

Table 4. Comparison of Calculated Values of K_{eff} of Experimental PuO_2-UO_2 Critical Assemblies

Case Number \ Source Spectrum	U-235	Pu-239
45	0.98645	0.98392
46	0.99625	0.99168
47	1.02306	1.01508
48	1.02273	1.01455
49	1.01051	1.00414
50	1.00083	0.99627
51	0.98533	0.99627
52	0.98913	0.98380
53	0.99927	0.99412
54	1.00813	1.00211
55	1.00637	1.00052
56	1.00579	0.99796
57	1.01178	1.00365
58	1.01292	1.00510
59	1.00909	1.00237
Average K_{eff}	: 1.00451	0.99883
Standard Deviation	: 0.01139	0.00930
Average $\|K_{eff}-1.0\|$	: 0.01032	0.00730

In calculations for mixed-oxide cores, coupled with the use of U-235 source spectrum, the average k_{eff} and the standard deviation become 1.0045 ± 0.0113 and the average deviation from unity becomes 0.0103.

In fact, fissile plutonium quantity in the selected mixed-oxide fuels is 3 times more than fissile uranium.

From this consideration, in calculations of mixed-oxide cores coupled with the use of Pu-239 source spectrum, the result gives the average k_{eff} of 0.9988 and the average deviation from unity of 0.0075. This represents an improvement.

The Cross Section Evaluation Working Group(CSEWG) evaluations[21] of the ENDF /B-IV concluded that the experimental k_{eff} is genrally overpredicted by 1 to 2 % for plutonium nitrate systems and underpredicted by~0.5 % for high moderator-to-fuel ratios up to 1.5 % for low moderator-to-fuel ratios in light water-moderated uranium lattices.

These biases have been confirmed by Kang & Hansen[22] or McCrosson[23] through benchmark analysis.

About 0.5~0.7 % underprediction of k_{eff} for the UO_2 system is very nearly the same as those of the CSEWG conclusion and the results of PuO_2-UO_2 system also show the same trend.

From the above results, a conclusion might be drawn that any bias remains in the library from ENDF/B-IV and the source spectrum greatly affects in the calculation of mixed-oxide system.

In determining whether a bias factor should be applied to the calculated value of k_{eff}, careful judgement is required.

4. Adjustment of Cross Section Data for UO_2 System

From the result of a previous discussion, 35 cases of UO_2 system (Case No. 1 through 35) were selected for data adjustment. The average k_{eff} and the standard deviation for these are 0.9929 ± 0.0086. Therefore, it will be assumed that calculated k_{eff} is always less than unity by more than 0.7 % for UO_2 fueled system.

In LEOPARD calculation, all resonance self-shielding is neglected except that in U-238. In MUFT routine for fast region, the self-shielding factor also includes the Doppler effect, since the cross section library of MUFT format contains no temperature dependence. The calculation of the resonance absorption is made in three steps: First the U-238 resonance escape probability is calculated for the lattice, then a self-shielding factor is obtained for U-238, finally the self-shielding factor is used to determine the fast spectrum and few group constants.

The microscopic scatterings of U-238 in the resonance region are important in the calculation of resonance integral. And then, these data used in the original LEOPARD library were the same values of 10.7 barns in the resonance regions, but since resonance data of U-238 from ENDF/B-IV were generated from resonance parameters, there are many resonance peaks. In fact, the LEOPARD selects a value of 45th fast group scattering data in order to calculate the above mentioned factors.

In the updated U-238 scattering data, the 45th group shows resonance peak and the value is 42.164 barns. This value is larger than the old data of 10.7 barns.

A bias factor on 0.7 % underprediction was applied in the LEOPARD calculation by adjusting a value of U-238 scattering. The 45th group scattering cross section was adjusted from 42.164 barns to 26.667.

The adjusted results are given in left side of Table 5. The average k_{eff} and the standard deviation are 0.9999 ± 0.0073 and the average deviation from unity is 0.0056. These values are greatly improved comparing with the values of 0.9929 ± 0.0086 in Table 3.

However, there are still some scattered values from unity. In order to reduce the scattered trend, another adjustment was tested.

In the fast region calculation of LEO

Table 5. Comparison of Calculated Values of Experimental UO_2 Critical Assemblies by Data Adjustments

Case Number \ Adj. Method	1st Method*	2nd Method**	Case Number \ Adj. Method	1st Method*	2nd Method**
1	0.98896	0.99596	19	0.99245	0.99510
2	0.99960	1.00245	20	0.98786	0.99039
3	1.00380	1.00331	21	0.98899	0.99132
4	1.01201	1.00769	22	0.98524	0.97998
5	1.01307	1.00826	23	1.00004	1.00146
6	1.00743	1.00218	24	1.00236	1.00041
7	0.99216	0.99700	25	1.01413	1.00800
8	1.00012	0.99813	26	0.99712	0.99069
9	0.99850	1.00197	27	0.99804	0.99940
10	1.01068	1.00742	28	1.00252	1.00164
11	1.00970	1.00641	29	1.00111	0.99892
12	1.00239	1.00005	30	0.99690	0.99770
13	0.99918	0.99734	31	0.99857	0.99763
14	0.99492	0.99404	32	0.99792	1.00063
15	0.99372	0.99295	33	1.00361	1.00100
16	0.99172	0.99115	34	1.00157	0.99986
17	1.01191	1.01007	35	1.00093	1.00378
18	0.99837	0.99868			
			Average K_{eff}	: 0.99993	0.99923
			Standard Deviation	: 0.00730	0.00611
			Average $\|K_{eff}-1.0\|$	: 0.00563	0.00459

* Changing the epithermal peak scattering of U-238 from 42.164 barns to 26.667

** Neglecting resonace scattering effects of U-238 and reducing of ν 0.8% in the thermal region

PARD, the resolved resonance absorption has explicit resonance treatment, but the resolved resonance scattering is not handled explicitly. In old library, resonance scatterings of a large number of nuclides were actually treated with constant values. By an input option of ETOG-3, it can be taken to be equal to the value in the first group above the resonance region.

With this treatment, all resonance scatterings of U-238 are determined as 12.067 barns. If resonance scattering data of U-238 in the updated library are substituted to 12.067 barns and the thermal ν of U-235 are reduced by 0.8 %, calculated results for UO_2 systems are also improved as shown in the right side of Table 5.

The average k_{eff} and the standard deviation are 0.9992 ± 0.0061 and the average deviation from unity is 0.0046. As the results of this adjustment, the scattered trend from unity of k_{eff} is greatly improved.

5. Conclusion

1) An updated ENDF/B-IV LEOPARD library was generated using ETOT-3 and ETOG-3 code system.

2) The applicability of the updated library was assessed through benchmark tests for many light water-moderated critical assemblies.

The statistical values for the ratios of the calculated k_{eff}'s to the measured are

0.9954±0.0152 for 44 UO_2-fueled cores, and 0.9988±0.0093 for 15 mixed-oxide(PuO_2-UO_2) plutonium-fueled cores.

In case of mixed-oxide system, it will be desirable to use mixed source spectrum of fissile materials.

3) In order to determine library bias from the result of benchmark tests, adjustment works were carried out by testing the statistical effect of k_{eff}'s on 35 UO_2-fueled system.

(1) Changing the epithermal peak scattering of U-238 from 42.164 barns to 26.667, the average k_{eff} and the standard deviation are 0.9999±0.0073.

(2) To reduce the scattered trend from unity, another adjustment was tested. Neglecting resonance scattering effects of U-238 and reducing ν of 0.8% in the thermal region, the standard deviation and the average deviation from unity are improved to 0.61% and 0.0046, respectively.

Thus, it is confirmed that the library from ENDF/B-IV, coupled with the use of LEOPARD code, leads to reasonable results for light water-moderated UO_2 fueled cores with the above adjustments.

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