Proceedings of the Korean Nuclear Society Spring Meeting
Kori, Korea, May 2000

Development and Validation of WIMS-D5 Library Based on JENDL-3.2

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Abstract

The WIMS-D5 library based on JENDL-3.2 has been generated and is being tested through analyses of the benchmark problems. Most of the material data in the 1986 WIMS-D library have been substituted for those of JENDL-3.2. The decay chains of fission products and actinides in the 1986 WIMS-D library were extended. The multiplication factors on the criticality benchmarks are slightly underpredicted with all libraries. The spectral indices in the lattices also agree with the measured values within the uncertainties of the experiments. The criticality predictions on the benchmark lattices with the new library are improved comparing with the results of the 1986 WIMS-D library.

1. Introduction

The WIMS-D[1] code 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 library[2] is based on old evaluated nuclear data and was empirically adjusted to achieve reasonable agreement between the calculated and measured integral parameters. The adjustments are not always justified by more accurate and recent experimental measurements. In view of the recently available new, or revised, evaluated nuclear data files, it was felt that the performance of WIMS-D could be improved by updating its library. Therefore, 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 library based on JENDL-3.2 has been produced and validated by analyzing the benchmarks such as TRX, BAPL, DIMP1A, WWER and WEDB1A lattices[5,6,7] at the Korea Atomic Energy Research Institute(KAERI).

2. Generation of WIMS-D5 Library

The cross section data were generated from JENDL-3.2 with a NJOY97.95 processing system[8]. The tolerances for linearizing and Doppler broadening of the cross section data were 0.2%. The epri-cpm 69 energy group structure was adopted and a weight function for generating the group constants from pointwise cross section data was the spectrum of British LWR[9] was chosen in the research coordination meeting for the WIMS Library Update Project sponsored by the IAEA. The British neutron current spectrum for transport correction was also used. The data included in the new WIMS-D library were generated as following.

(a) Fission Spectrum

Only one fission spectrum is required in the WIMS-D library. The spectra of U-235, U-238 and Pu-239 were calculated and weighted by 57%, 8% and 35% for a single spectrum, respectively. Table 1 shows the spectra at the 27 energy groups in the WIMS-D library.

(b) Q value

The Q values in the WIMS-D library, which are the deposited energy in the system, are dependent on the system analyzed. The total deposited energy(Q_T) can be represented as

$$Q_T = Q_{eff.} + (\nu_T - 1) \times Q_c ,$$

where the recoverable energies per fission reactions, $Q_{eff.}$, were obtained from JENDL-3.2 and the released energy per neutron capture, Q_c, is 6.1 MeV. The $Q_{eff.}$ values in JENDL-3.2 are represented in Table 2.

(c) Burnup chains of fission products and actinides

The burnup chains in the 1986 WIMS-D library were extended. The solid lines in Figure 1 are the burnup chains of the 1986 library and the extended chains in the new library based on JENDL-3.2 are represented by dashed lines. The (n,α) reaction chains for most of the actinides are added. 48 fission product nuclides from the actinides were treated explicitly. The fission product yield data in JENDL-3.2 were used for Th-232, U-233, -235, -236, -238, Np-237, Pu-239, -240, -241 and –242, and for the others in ENDF/B-VI.

(d) Cross section data

Most of the cross section data of the material in the 1986 WIMS-D library have been substituted for JENDL-3.2 data. The cross sections of a pseudo fission product were calculated from 86 fission products from U-235(57%), U-238(8%) and Pu-239(35%). The absorption and transport cross sections of a pseudo material generated from the JENDL-3.2 data are compared

with those of ENDF/B-VI in Figure 2. The P1 scattering matrix data were produced from ENDF/B-VI.

3. Benchmark Calculations

The criticality benchmarks for the validation of the new library are the TRX-1, -2, -3, BAPL-1, -2, -3, and DIMP-1A lattices. The TRX lattices are light water moderated uranium metal fuel cores in a hexagonal geometry. The BAPL and DIMP1A lattices are light water moderated uranium oxide cores in a square geometry. The multiplication factors and spectral indices were calculated and compared with the measured values. The integral parameters are defined as following.

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

δ^{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 criticality calculations were performed and the results were compared with the measurements of WWER-type UO_2-H_2O lattices. The measured material bucklings were given as input. A critical buckling search was also carried out for direct comparison with the experimental values. The lattices are identified as P/E/CB/T, where

P : lattice pitch [cm]

E : atomic enrichment [at. %]

CB : boron concentration [g H_3BO_3/Kg solution]

T : temperature [C].

The OECD/NEA burnup credit benchmark part-1A(criticality prediction) is a numerical one. The reference solution was obtained by averaging 25 sets of results produced by 19 participating laboratories using different data libraries and codes. The benchmark effectively measures the influence of the cross sections on the reactivity change while varying burnup and fuel cooling time.

4. Results and Discussion

The calculated multiplication factors with the other libraries are compared with the measured values in Table 3 ~ 8. The k-effective values with all libraries are slightly underpredicted. One of the reasons seems to be that the spectrum in the resonance region is too soft and therefore shifted into the region of a less capture to fission ratio. The spectral indices in the lattices also agree with the measured quantities within the uncertainties of the experiments. The results with the library based on JENDL-3.2 are comparable with the others. The results of WWER-type lattice are compared with the measurements in Table 9. The multiplication factors for 17 cases were calculated and the results agree with the measurements within a maximum of 1.4% in case 15. The results of a critical buckling search also show a difference from the

measurement by 6.8% in case 15. The predictions of criticality on the WWER lattice with the library based on JENDL-3.2 show overestimation in most cases. For comparing with the results of the ENDF/B-VI.5-based library, the difference in k-eff from the measurements is also presented. Table 9 shows the underestimation in k-eff with the ENDF/B-VI-based library and the difference from the results with JENDL-3.2-based library is about 500 ~ 1,000 pcm.

The calculated results of the WEDB1A NEA burnup credit benchmark are represented in Table 10. This benchmark is a numerical one. Eleven cases are investigated and in the benchmark 2*sigma uncertainties are quoted. To eliminate systematic errors, the differences in the k-eff relative to a case with fresh fuel are considered. The results with the new library agree well in the view of the uncertainty of the reference solution. The results with the updated library show improvements comparing with those of the 1986 library. The results with the updated WIMS-D library are at least as good compared to what is predicted by the other codes and libraries because it is possible that the reference results are biased.

5. Conclusions

The WIMS-D5 library based on JENDL-3.2 has been generated and is being tested through analyses of the benchmarks. With the updated library, the predictions of criticality and spectral indices on the benchmark lattices are very good. The results with the JENDL-3.2 based library show improvements comparing with those of the 1986 WIMS-D library. The new library based on JENDL-3.2 is not completed yet. The research for improvements of burnup chains and resonance treatments will continue. The material identification numbers will be fixed and the additional benchmark tests will be carried out.

Acknowledgement

This work to update the WIMS-D library is supported by the Ministry of Science and Technology of Korea. This work is also sponsored by the IAEA. The authors greatly appreciate the assistance of Dr. A. Trkov in Slovenia.

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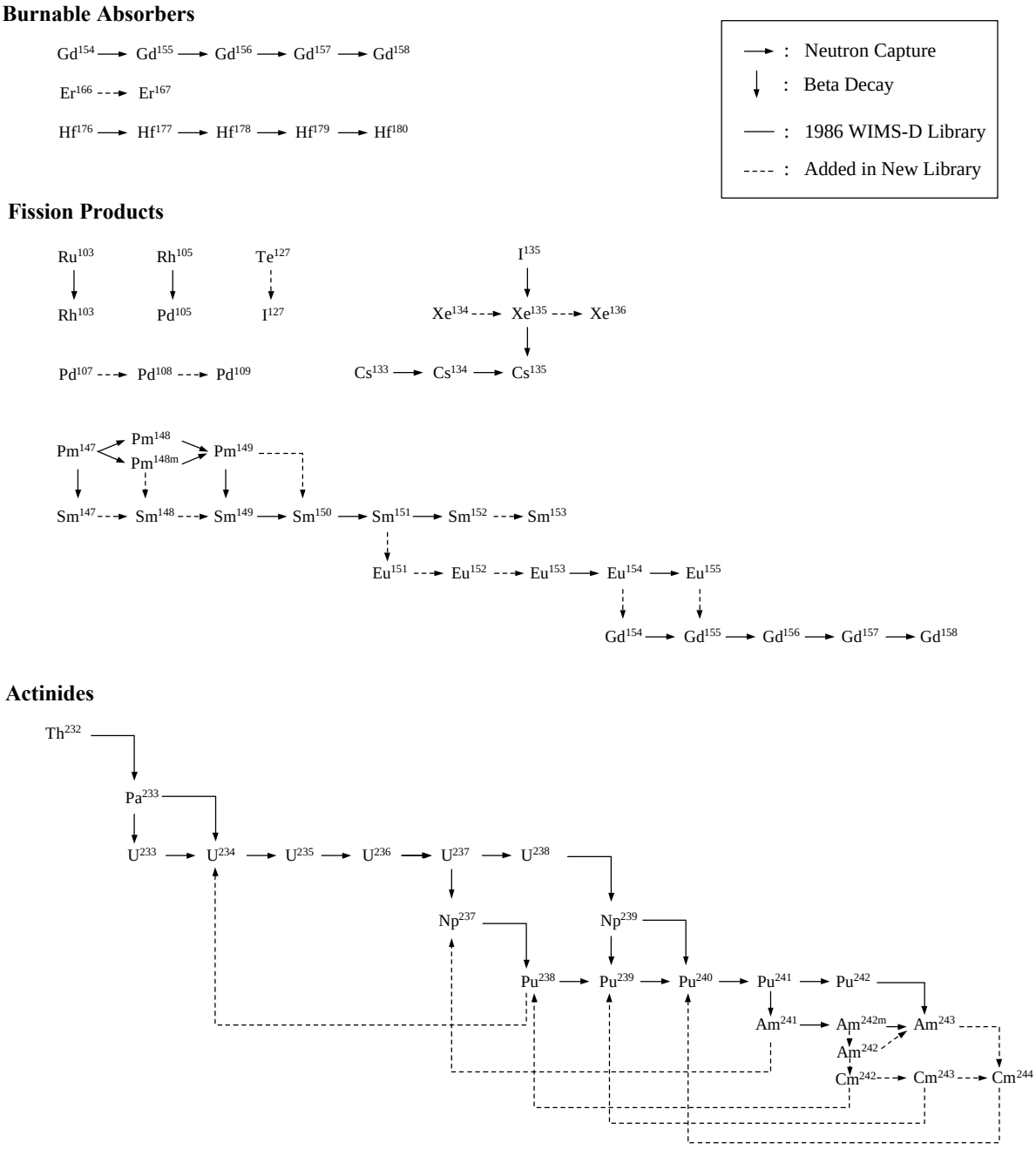

Figure 1. The Burnup Chains of Fission Products and Actinides in the WIMS-D Library

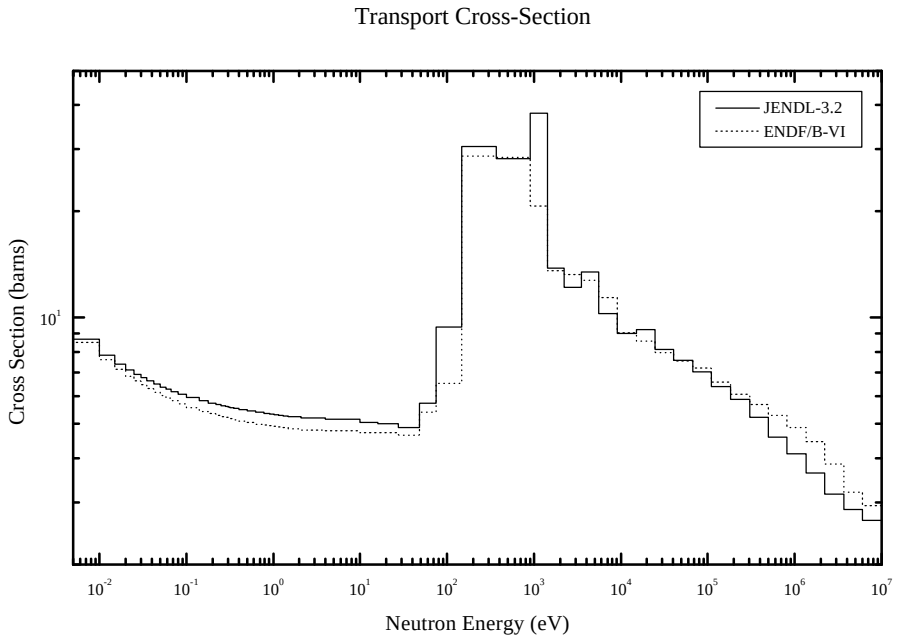

Figure 2. The Cross Sections of a Pseudo Fission Product in the WIMS-D Library

Table 1. Fission Spectrum in the Library

Groups	Fission Spectra
1	2.54367537E-02
2	1.11181725E-01
3	2.15993776E-01
4	2.35126315E-01
5	1.77651609E-01
6	1.11392130E-01
7	6.23231636E-02
8	3.15159857E-02
9	1.52716095E-02
10	7.38905356E-03
11	3.53293732E-03
12	1.67810845E-03
13	7.94310073E-04
14	3.74687361E-04
15	1.78306610E-04
16	7.86050401E-05
17	3.98827781E-05
18	2.02175132E-05
19	1.02279262E-05
20	7.87650496E-06
21	2.02684330E-06
22	4.47697520E-07
23	1.25461985E-07
24	7.27301895E-08
25	3.17786049E-08
26	1.26591081E-08
27	8.22346880E-10

Table 2. The Recoverable Energy per Fission

Actinides	$Q_{eff.}$ values (MeV)
90-Th-232	185.379
91-Pa-233	187.209
92-U –233	190.
92-U –234	190.
92-U –235	193.109
92-U –236	190.
92-U –237	200.
92-U –238	190.
93-Np-237	190.
93-Np-239	190.
94-Pu-238	195.
94-Pu-239	200.
94-Pu-240	197.019
94-Pu-241	201.659
94-Pu-242	195.
95-Am-241	195.
95-Am-242m	200.
95-Am-243	200.
96-Cm-242	200.
96-Cm-243	200.
96-Cm-244	200.

Table 3. 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	1.18009*	0.99301+	1.028	0.988	1.038	1.005
WIMS1986	1.18686	0.99314	1.017	0.992	1.067	0.990
ENDF/B-VI.5	1.17562	0.98774	1.029	0.990	1.053	1.010
JEF-2.2	1.17831	0.99163	1.027	0.995	1.037	1.009

* Calculated Value

\+ Calculated/Experimental Value

Table 4. 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	1.16602	0.99444	1.016	0.976	1.012	0.998
WIMS1986	1.17142	0.99482	1.004	0.980	1.040	0.986
ENDF/B-VI.5	1.16192	0.99007	1.016	0.977	1.019	1.003
JEF-2.2	1.16339	0.99235	1.014	0.982	1.007	1.003

Table 5. 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	1.14498	0.99931	1.014	0.980	0.979
WIMS1986	1.14873	0.99887	1.010	0.985	1.008
ENDF/B-VI.5	1.13913	0.99374	1.017	0.980	0.985
JEF-2.2	1.14219	0.99749	1.013	0.986	0.974

Table 6. 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	1.14917	0.99899	1.047	0.988	0.940
WIMS1986	1.15247	0.99820	1.044	0.994	0.969
ENDF/B-VI.5	1.14369	0.99388	1.049	0.987	0.941
JEF-2.2	1.14630	0.99708	1.046	0.993	0.934

Table 7. 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	1.13518	0.99942	1.017	0.994	0.947
WIMS1986	1.13797	0.99868	1.013	1.002	0.977
ENDF/B-VI.5	1.13020	0.99488	1.019	0.992	0.947
JEF-2.2	1.13219	0.99730	1.015	0.998	0.940

Table 8. Comparison of C/E Integral Parameters in the DIMP-1A Lattice

Quantities	k-inf.	k-eff.	ρ^{28}	C^*
Exp. (%Err.)		1.00000 (0.1)	0.0962 (3.3)	0.647 (0.46)
JENDL-3.2	1.27048	1.00529	0.899	1.003
WIMS1986	1.26654	0.99393	0.932	0.997
ENDF/B-VI.5	1.25594	0.99193	0.918	1.012
JEF-2.2	1.26068	0.99789	0.901	1.009

Table 9. The Results of WWER-Lattice Criticality Benchmarks (B(1) corrected solution)

No.	Lattice	K-inf.	K-eff.	K_{eff} -1.0[pcm]		Cal. $B^2[1/m^2]$ Diff. $[1/m^2]$ Diff. [%]	Exp. $B^2[1/m^2]$ Std. $[1/m^2]$ Std. [%]
				JENDL -3.2	ENDF/B -VI.5		
1	1.27/3.6/0.0/20 *	1.41997	1.01208	1209	400	102.07 3.83 3.90	98.24 0.99 1.01
2	1.27/3.6/0.0/80	1.41297	1.00045	46	-793	96.68 0.13 0.14	96.55 1.29 1.34
3	1.27/3.6/0.0/130	1.40464	0.99855	-145	-1016	89.83 -0.44 -0.48	90.27 0.91 1.01
4	1.27/3.6/4.0/20	1.30968	1.00348	348	-426	77.08 1.06 1.39	76.02 0.14 0.18
5	1.27/3.6/4.0/80	1.30634	1.00461	461	-348	73.42 1.35 1.88	72.07 0.21 0.29
6	1.27/3.6/4.0/130	1.30282	1.00417	418	-425	68.79 1.16 1.71	67.63 0.20 0.30
7	1.27/3.6/5.8/20	1.26604	1.00605	606	-152	66.76 1.82 2.81	64.94 0.26 0.40
8	1.27/3.6/5.8/80	1.26400	1.00728	729	-66	63.80 2.11 3.41	61.69 0.20 0.32
9	1.27/3.6/5.8/130	1.26219	1.00376	377	-450	60.05 1.03 1.74	59.02 0.13 0.22
10	1.10/3.6/0.0/20	1.31018	1.00470	470	-477	65.72 1.21 1.88	64.51 0.34 0.53
11	1.10/3.6/0.0/80	1.29938	0.99390	-609	-1573	61.61 -1.54 -2.45	63.15 0.48 0.76
12	1.10/3.6/0.0/130	1.28648	0.98964	-1036	-2015	56.49 -2.50 -4.24	58.99 0.29 0.49
13	1.10/3.6/1.0/20	1.29609	1.00414	415	-523	62.85 1.07 1.72	61.78 0.34 0.55
14	1.50/3.6/0.0/20	1.45020	1.00209	210	-449	121.45 0.76 0.63	120.69 0.53 0.44
15	1.50/3.6/4.0/20	1.26538	1.01411	1411	785	74.16 4.74 6.82	69.42 0.15 0.22
16	1.50/1.6/0.0/20	1.18230	1.00103	104	-347	48.62 0.26 0.54	48.36 0.49 1.01
17	1.50/4.4/0.0/20	1.49979	0.99697	-303	-1012	135.62 -1.18 -0.86	136.80 0.51 0.37

* Pitch/enrichment/boron concentration/temperature

Table 10. The Results of WEDB1A - NEA Burnup Credit Benchmark (Part-1A Criticality Prediction)

CASE	K-ref.	Calulated K-ref.		Delta K-ref.*	Delta K-cal.	
		New Lib.	1986 Lib.		New Lib.	1986 Lib.
1	1.43780	1.44383	1.44441	0	0	0
	1750[a]	602[b]	660	0	0	0
		0.42[c]	0.46		0.00	0.00
2	1.14020	1.14007	1.15739	-29760	-30376	-28701
	1689	-13	1719	1340	-616	1058
		-0.01	1.51		2.07	-3.56
3	1.06380	1.06295	1.08155	-37400	-38088	-36285
	1700	-85	1774	1540	-688	1114
		-0.08	1.67		1.84	-2.98
4	1.24560	1.24934	1.24726	-19220	-19449	-19715
	1070	373	165	970	-229	-495
		0.30	0.13		1.19	2.58
5	1.18850	1.19134	1.18850	-24930	-25248	-25590
	1100	284	0	1070	-318	-660
		0.24	0.00		1.28	2.65
6	1.11230	1.11282	1.12884	-32550	-33100	-31557
	1640	52	1653	1490	-550	993
		0.05	1.49		1.69	-3.05
7	1.02400	1.02367	1.04025	-41380	-42015	-40415
	1560	-32	1625	1470	-635	964
		-0.03	1.59		1.54	-2.33
8	1.22840	1.23303	1.23029	-20940	-21080	-21412
	1090	462	188	990	-140	-472
		0.38	0.15		0.67	2.25
9	1.16570	1.16887	1.16513	-27210	-27496	-27928
	990	316	-57	1140	-286	-718
		0.27	-0.05		1.05	2.64
10	1.26350	1.26667	1.26579	-17430	-17715	-17861
	1080	317	229	1000	-285	-431
		0.25	0.18		1.64	2.48
11	1.25660	1.25993	1.25881	-18120	-18389	-18560
	1090	333	220	970	-269	-440
		0.27	0.18		1.49	2.43

* Delta K = K(Case n) - K(Case 1)

[a] Uncertainty (2 sigma) for reference

[b] Difference from reference for cal.

[c] Difference(%)