Benchmarking of ^{232}Th from JEFF-3.1

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1. Background

The purpose of the benchmarking exercise was to validate the new ^{232}Th and ^{233}U evaluations in the JEFF-3.1 library in comparison with ENDF/B-VI.8 data and with the new ENDF/B-VII.b2 library, which includes the evaluated nuclear data file for ^{232}Th developed through the IAEA co-ordinated research project (CRP) on “Evaluated Nuclear Data Files for the Th-U Fuel Cycle”. The work was performed under the bilateral agreement between the Ministry of higher education, science and technology of Slovenia (MVZT) and Commissariat à l'Énergie Atomique (CEA), France.

2. Scope

Benchmarks from the ICSBE Handbook that were considered in the analysis are shown in Table 1. The RBMK benchmarks were not analysed because it was felt their sensitivity to thorium data is not very high. Benchmarks in which thorium appears only as an impurity were also excluded.

Table 1.: List of thorium-bearing lattices in ICSBEP.

Ident	Cases		Description
HEU-MET-FAST-068	1	KBR22	KBR22 (U/Th metal, polyethylene)
HEU-MET-INTER-008	1	KBR23	KBR23 (U/Th metal, polyethylene)
IEU-COMP-FAST-002	1	KBR18	KBR18 (90%235UO2+Th metal+36%235UO2)
IEU-COMP-INTER-001	1	KBR19	KBR19 (90%235UO2+Th metal+36%235UO2, polyethylene)
	1	KBR20	KBR20 (90%235UO2+Th metal, polyethylene)
IEU-COMP-THERM-005	1	KBR21	KBR21 (36%235UO2+Th metal, polyethylene)
PU-MET-FAST-008	1	THOR	THOR Pu sphere/Th-reflector
HEU-COMP-THERM-015	1	LWBR SB-1	LWBR SB-1 (93%235UO2+ZrO2, ThO2 blanket)
	1	LWBR SB-5	LWBR SB-5 (93%235UO2+ZrO2, ThO2 blanket)
U233-COMP-THERM-001	1	LWBR SB-2	LWBR SB-2 (97%233UO2+ZrO2, ThO2 blanket)
	1	LWBR SB-2½	LWBR SB-2½ (97%233UO2+ZrO2, no blanket)
	1	LWBR SB-3	LWBR SB-3 (97%233UO2+ZrO2, UO2+ThO2 blanket)
	1	LWBR SB-4	LWBR SB-4 (97%233UO2+ZrO2, UO2+ThO2 blanket)
	1	LWBR SB-6	LWBR SB-6 (97%233UO2+ZrO2, ThO2 blanket)
	1	LWBR SB-7	LWBR SB-7 (97%233UO2+ZrO2, UO2+ThO2 blanket)
LEU-COMP-THERM-060	10	RBMK	RBMK (Th absorbers, cases 19-28)
U233-SOL-THERM-006	1	ORCEF	ORCEF (Th as impurity only)
U233-SOL-THERM-008	1	ORNL	ORNL (Th as impurity only)
U233-SOL-THERM-009	1	ORNL	ORNL (Th as impurity only)
U233-SOL-THERM-012	1	ORCEF	ORCEF (Th as impurity only)
U233-SOL-THERM-013	1	ORCEF	ORCEF (Th as impurity only)

In addition, the benchmark from the SINBAD database on the IPPE leakage spectrum measurement from thorium sphere with a D-T source was considered.

The MCNP5 Monte Carlo code with various data libraries was used in the analysis. The inputs for MCNP5 were taken from the ICSBEP handbook or the SINBAD specifications, but the number of particle histories and the number of batches for k_{eff} determination were increased so that the statistical error in the calculations was negligible compared to experimental uncertainties. Material composition data were also changed where necessary to replace elemental number densities with the corresponding isotopic ones. Sensitivity analysis on the source data libraries was performed. Most of the libraries were available from the MCNPDATA package distribution. The ACE files from ENDF/B-VII.b2 library were obtained from NNDC, Brookhaven. The change in the average number of neutrons per fission at thermal energies for ^{233}U as recommended for ENDF/B-VII.b3 was done locally. Additional libraries and ^{232}Th and ^{233}U files in ACE format were generated at the IAEA and at IJS. The following libraries were considered in the analysis

ENDF/B-VI Rel.8	The ".62c" series of materials in the ACTI files of the MCNPDATA set.
ENDF/B-VII.b2+	The ENDF/B-VII.b2 library generated at NNDC, Brookhaven, with correction for the neutron yield flag in the TYR block. The only change (done locally) for ENDF/B-VII.b+ is the average number of neutrons per fission of ^{233}U.
JEFF-3.1	The library generated at the NEA Data Bank based on JEFF-3.1 data.
ADS	Reference library for ADS from the IAEA based on JEFF-3.1 data, but containing a limited number of materials (the rest taken from the default ACE library based on ENDF/B-VI data).

3. Results

The results are presented as the differences between the calculated multiplication factor k_c and the measured one k_m in units of parts per 100 000 (pcm). Separate plots for each set of benchmarks are presented.

KBR benchmarks

In the KBR series of benchmarks, cases 22 and 23 are critical configurations; cases 18 to 21 are k_∞ measurements with progressively softer spectra and are highly sensitive to ^{232}Th data. In Figure 1 the sensitivity of the results on different libraries is presented. The maximum spread in the results with ENDF/B-VI.8 data is around 7000 pcm. The biggest outliers are KBR-18 and 21 with hardest and softest spectra, respectively. The use of JEFF-3.1 data does not improve the agreement between measurements and calculations. The improvement using ENDF/B-VII.b+ data is significant; the maximum spread of the results is reduced to about 3000 pcm, although the two outliers are still slightly outside the 2σ uncertainty interval. The influence of the new ^{232}Th data alone is shown in Figure 2, confirming that these data are chiefly responsible for the improvement.

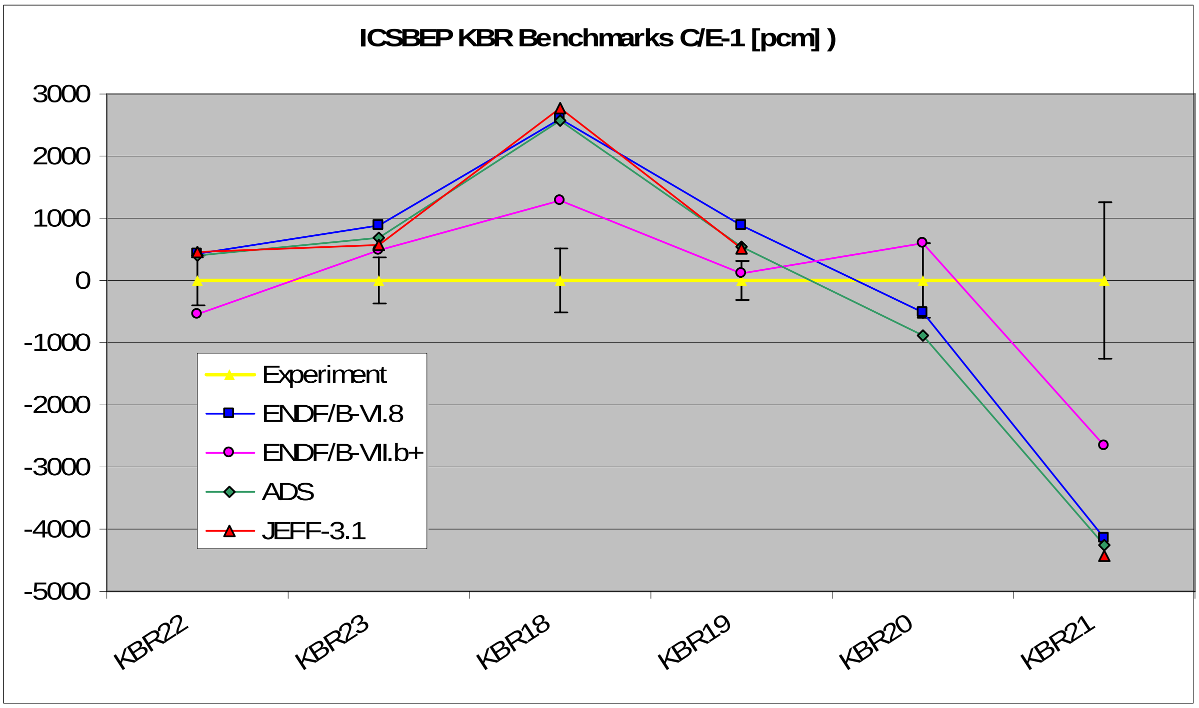

Figure 1.: Results of calculations for the KBR series of benchmarks with different libraries

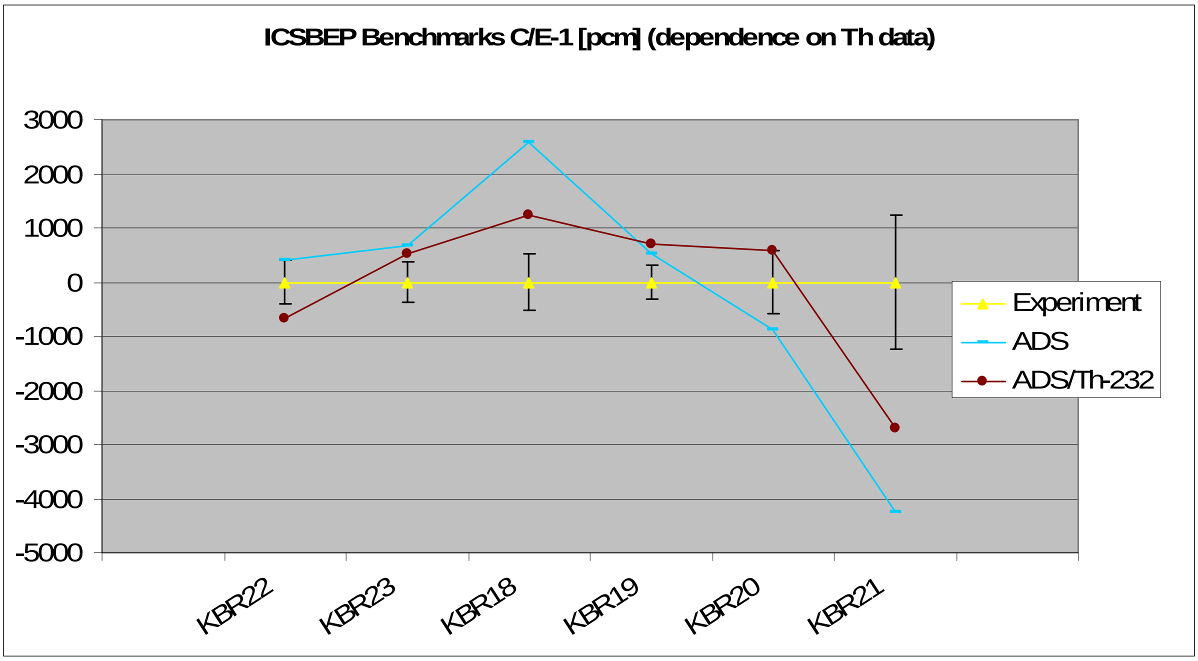

Figure 2.: Sensitivity of the KBR benchmarks on ^{232}Th data (ENDF/B-VI.8 vs. ENDF/B-VII.b+)

SB-n benchmarks

The SB-n series of benchmarks are thermal lattices with thorium blanket and either ^{235}U (SB-1,5) or ^{233}U (other SB lattices) fissile component in zirconium matrix fuel. As seen from Figure 3, the use of JFFF-3.1 data does not improve the agreement between measurements and calculations compared to ENDF/B-VI. The results with the new ENDF/B-VII.b+ data lie completely within the 1σ uncertainty interval, except for lattice SB-6, which is the only outlier, but still well within the 2σ uncertainty band.

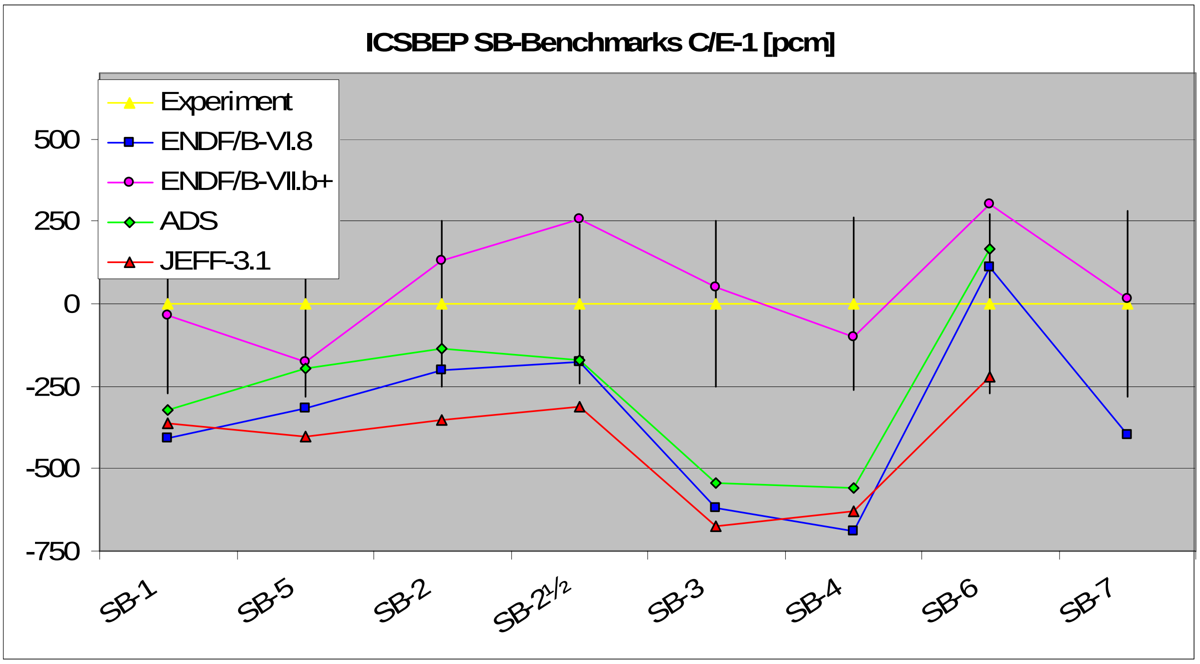

Figure 3.: Results of calculations for the SB-n series of benchmarks with different libraries

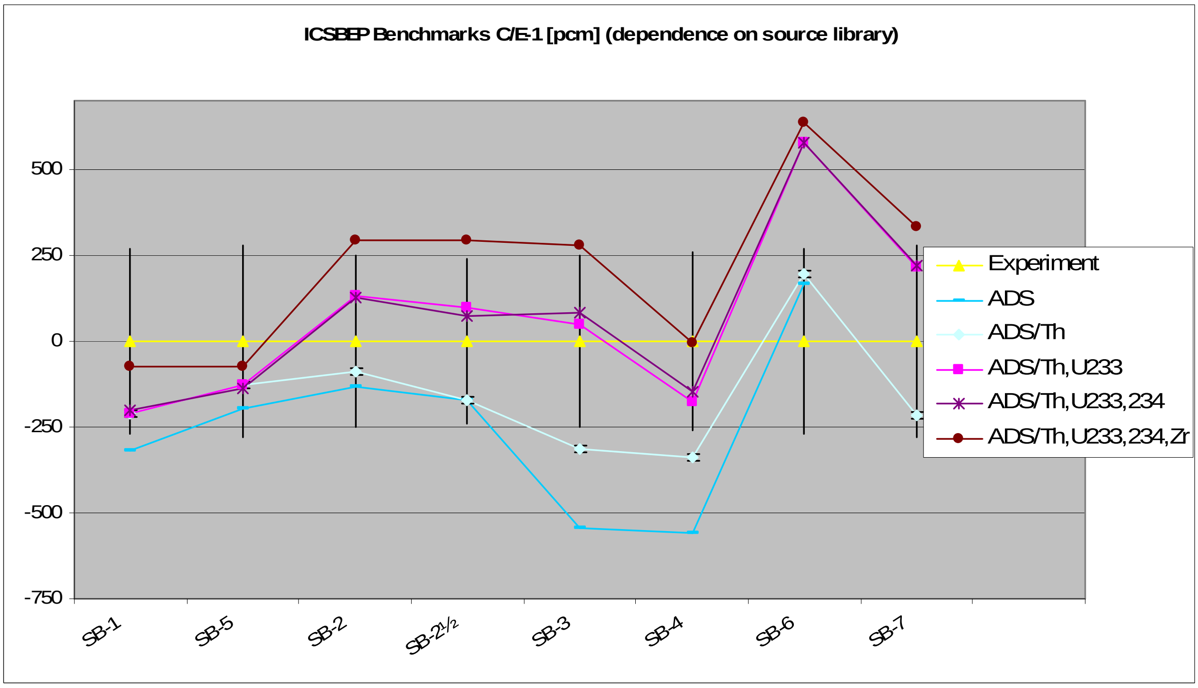

Figure 4.: Sensitivity of the SB-n benchmarks on nuclear data

Sensitivity of SB benchmarks to nuclear data

Sensitivity to nuclear data of individual nuclides is quite revealing. Starting arbitrarily with the base calculation using ADS library (where ^{232}Th data were taken from ENDF/B-VI.6), the data for ^{232}Th, ^{233}U, ^{234}U and zirconium were replaced with the data from ENDF/B-VII.b2. The results in Figure 4 show strong sensitivity of SB-3 and SB-4 lattices to ^{232}Th data. The new IAEA evaluation for ^{232}Th greatly reduces the scattering in the results. The addition of ^{233}U data from ENDF/B-VII.b2 introduces a distinctly positive bias in the lattices that bear ^{233}U, while the impact of ^{234}U is practically negligible.

The data for zirconium, which is the matrix material in the fuel, also produce a positive bias, which together with ^{233}U data cause the over prediction of reactivity. The reduction of the average number of neutrons per fission in ^{233}U of ENDF/B-VII.b+ (to be in agreement with the new evaluation of the Standards) completely removes the bias, as evident from the results with ENDF/B-VII.b+ data in Figure 3.

Sensitivity to benchmark uncertainties

There is some degree of uncertainty in control blade positions in the benchmark description. Originally the experimenters envisaged control blade position to be determined from the measured bucklings B_z^2 and Equation 1:

$$B_z^2 = \left[\frac{\pi}{H_C + 2\delta} \right]^2 , \qquad \textit{Equation 1}$$

where H_C is the control blade position and δ is the extrapolation distance, determined to be 8 cm from the benchmark case SB-2½, where the control blade position was more accurately known. When analysing the benchmarks this procedure of determining control blade positions was found highly questionable and sensitive to the choice of the measured buckling values, namely:

- *either* buckling averaged over the seed region of the core,
- *or* buckling taken from the centre-most region (Region I) of the core.

The finally adopted value was the average of the two buckling choices, averaged over all cases (except SB-2½) and fixed for all cases, except SB-2½ in which the original experimenters' recommendation could be followed without ambiguities. The final control blade insertion depths were 3.00±0.75 cm for SB-2½ and 3.285±1.695 cm for all other cases. Detailed results in Table 2 give differences from the adopted control blade positions D_i for the two choices of bucklings and the average of the two for each benchmark case. The following observations can be made:

- Values of D_i differ significantly for the two choices of bucklings.
- The average values are close to the adopted and well within the assigned uncertainty, except for case SB-6, where a deeper control blade insertion would be favoured. This benchmark case is precisely the one that seems to be the outlier in Figure 3.

Table 2: Differences in control blade position D_i from adopted, using different assumptions for buckling.

Lattice	D_i(Seed)	D_i(Reg.I)	D_i(Aver.)
SB-1	-0.21	0.20	-0.01
SB-5	0.35	0.33	0.34
SB-2	0.31	-0.12	0.09
SB-2½	0.00	0.00	0.00
SB-3	-0.49	-0.93	-0.71
SB-4	-1.23	-1.27	-1.25
SB-6	2.15	1.79	1.97
SB-7	-0.87	0.01	-0.43

Reliability of control blade positions could be improved and uncertainties reduced by explicit calculations, varying assigned control rod positions and matching the measured axial flux profiles.

Although this information is discussed in the benchmark description, the measured data are not provided.

Thor benchmark

The Thor benchmark is a thorium-reflected plutonium sphere. Interpretation of the results depends strongly on nuclear data for plutonium. Predicted reactivity is 224 pcm above the benchmark value, but this should be considered with reference to the results for bare plutonium sphere benchmarks, which is outside the present scope of work.

IPPE sphere leakage current benchmark

Using the SINBAD model the results with the ENDF/B-VII.b+ data agree with the measurement to about 20%. The main difference is in the low-energy tail of the spectrum, where the (n,3n) reaction has the dominant contribution. A reduction of the (n,3n) cross section near threshold would improve the results. This benchmark is strongly influenced by the old processing error in generating the ACE file for ^{232}Th with older versions of NJOY. Without the correction the agreement between measured and calculated spectra at low energies is perfect, but a "hole" in the spectrum is observed between 2 and 6 Mev. The spectra are shown in Figure 5.

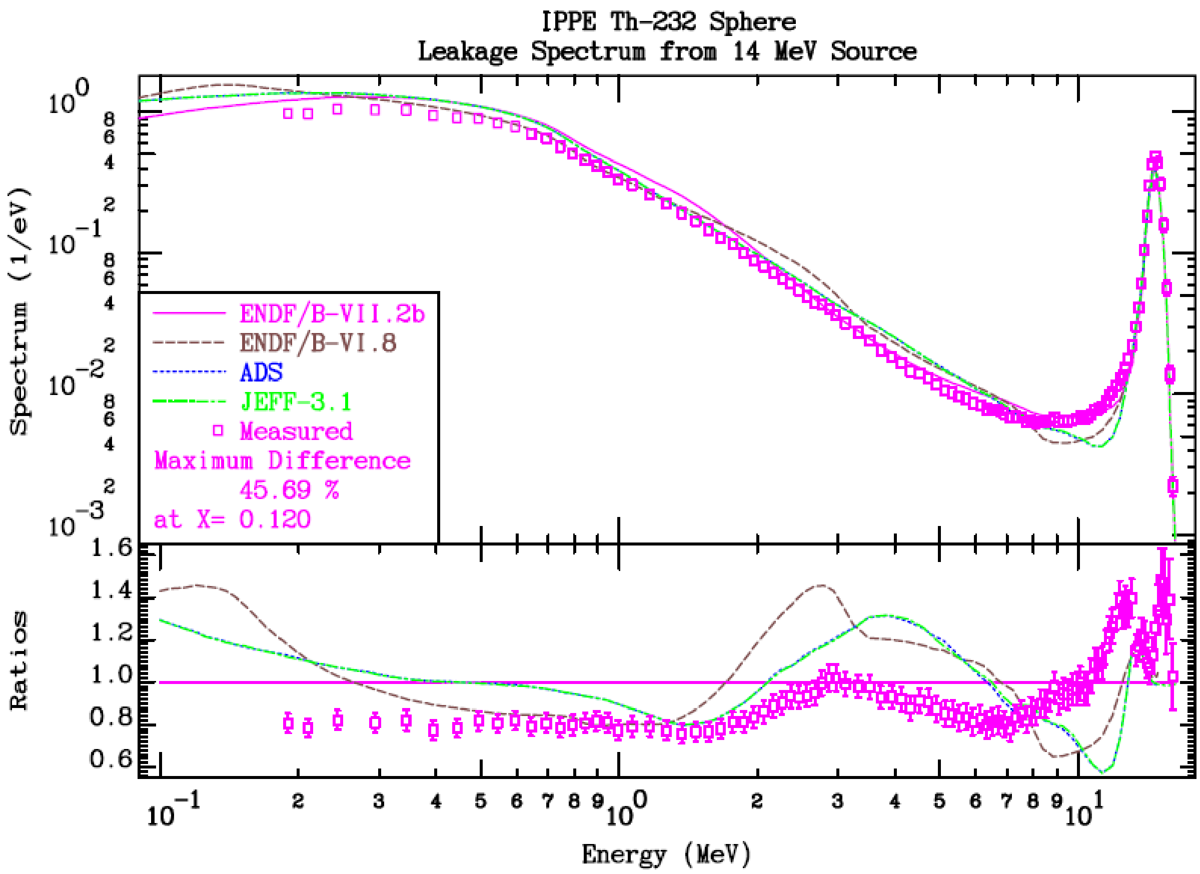

Figure 5.: Leakage spectrum from the IPPE thorium sphere with D-T source.

Apart from the possible cause of the discrepancy between measurement and calculation due to the cross sections, the benchmark model itself is an approximation to the real configuration. It does not model the collimator explicitly. Instead, the benchmark recommendation is to use the source spectrum without the sphere in place to simulate the resolution broadening response function. Unfortunately the available information on the benchmark is insufficient to improve the model.

Conclusions

The results of benchmark calculations are summarised in Table 2. The KBR benchmarks indicate a clear improvement only when the ENDF/B-VII.b2+ data are used, although the discrepancies for the lattices with the hardest and the softest spectrum still slightly exceed the 2σ level; experimental uncertainties are large and a possible problem with the measurement or its interpretation cannot be ruled out. The analysis of the SB-n benchmarks with JEFF-3.1 data shows no improvement compared to ENDF/B-VI. The results with ENDF/B-VII.b2 data are within the experimental uncertainties, except for the SB-6 lattice, which lies slightly outside. Further improvement and reduction of experimental uncertainties seems possible by refining the procedures for determining the control blade positions in the SB-n benchmark cases. The results for the Thor benchmark are slightly high but should be considered in combination with the results for bare plutonium sphere benchmarks. The IPPE thorium sphere leakage benchmark tests the data at higher energies. Before assigning the discrepancies between measurements and calculations to the data, the effect of an explicit model of the collimator should be investigated.

Table 3.: Differences between calculated and measured multiplication factor in units 10^5(C/E-1).

Case	k-eff	Unc. [pcm]	JEFF-3.1	ENDF/B-VI.8	ENDF/B-VII.b+
THOR	1.00000	60	224	567	-187
KBR22	1.00010	410	451	434	-545
KBR23	1.00080	360	584	874	493
KBR18	0.96900	516	2761	2593	1273
KBR19	0.98000	306	508	882	121
KBR20	1.01400	592	-937	-527	602
KBR21	0.96400	1245	-4439	-4154	-2662
SB-1	1.00060	270	-365	-410	-34
SB-5	1.00150	280	-400	-316	-178
SB-2	1.00150	250	-352	-204	132
SB-2½	1.00000	240	-312	-175	255
SB-3	1.00070	250	-675	-618	51
SB-4	1.00150	260	-636	-690	-102
SB-6	0.99950	270	-185	111	304
SB-7	1.00040	280	-	-397	15