

## Assessment of Standard Point-wise Neutron Data Libraries for Criticality Safety Analysis with a Monte Carlo Code

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### Abstract

This study addresses the assessment of standard continuous-energy neutron data libraries using the Monte Carlo radiation transport code MCNPX for light water reactor criticality safety applications based on a suite of low-enriched, thermal, compound uranium benchmarks and represents a continuation of previously performed analysis using the JEF-2.2 and JENDL-3.3 nuclear data libraries.

The new work enhancing the previous study includes the application of the ENDF/B-6.8 neutron data library and employs the most recent official release of the code (MCNPX-2.5.0) with an improved  $S(\alpha,\beta)$  thermal neutron scattering treatment.

Particular attention is paid to the analysis of the spectrum-related characteristics of the modeled critical experimental configurations to define the range of applicability of the reported estimates of lower tolerance bounds for  $k_{\text{eff}}$ . Inspection of trends in  $k_{\text{eff}}$  versus the spectrum-related characteristics or design parameters has also been performed.

**KEYWORDS:** *criticality safety assessment, MCNPX, standard libraries*

## 1. Introduction

The paper is focused on assessment of the standard neutron data libraries JEF-2.2 [1], JENDL-3.3 [2] and ENDF/B-6.8 [3], distributed by the NEA/OECD Data Bank, for LWR criticality safety applications with the MCNPX code [4]. For this purpose, benchmark calculations were performed for a suite of benchmarks [5] from the International Handbook of Evaluated Criticality Safety Benchmark Experiments [6], selected based on their similarity to designs found in today's LWR compact storage pools and transport casks.

The previous studies were mostly concerned with the discussion of the applicability of the  $k_{\text{eff}}$  lower tolerance bounds (LTB) estimates based on the assumption of normality of the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  distribution. In this paper we present detailed studies of spectrum-related characteristics of the modeled benchmark configurations, accompanied by an analysis of trends in the calculated  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  samples. We note that significant trends, if present, have to be taken into account for the establishment of a subcriticality safety limit [7].

The present studies form a compulsory step towards the establishment of a methodology for criticality safety evaluation by demonstrating the adequacy of the set of calculated benchmark experiments with respect to the real storage pools to be analyzed.

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The methodology for criticality safety evaluations using the MCNPX code is currently under development at PSI within the STARS project [8], while the existing approach is based on the deterministic in-house BOXER code and associated group-wise library.

## 2. Methodology

As the methodology applied is the same as in the previous studies [6] and as such has been described earlier, it is pertinent to present just a short summary here. Based on their similarity to the designs of current-day LWR compact storage pools and transport casks, suitable evaluated benchmark experiments were selected from the “International Handbook of Evaluated Criticality Safety Benchmark Experiments” [5]. Both the selection procedure and the characteristics of the benchmarks are discussed in [6]. The number of independently evaluated experiments selected for the analysis amounts to 15, and the total number of benchmark cases equals 106.

From the previous stage of the studies [6] the following hypothesis emerged: Non-specified experiment/evaluation-related biases in the  $k_{\text{eff}}^{\text{bench}}$  values could potentially explain the observed deviation of the distribution of the ratio between calculated and experimental results from normal, particularly if very accurate Monte Carlo criticality calculations are performed. Uncertainties of the point-wise neutron cross sections could as well be system or spectrum-correlated. This puts into question the reliability of an analysis based on the assumption of normality of the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  distribution, bearing in mind that this assumption is frequently used for practical criticality safety evaluation due to its easiness and flexibility of application.

Because of these concerns, we once again use in the present study the distribution-free estimates for  $k_{\text{eff}}$  LTB to check the estimates based on the assumption of normality of calculated results. Fortunately, the differences between these two approaches are shown to be insignificant from the practical point of view.

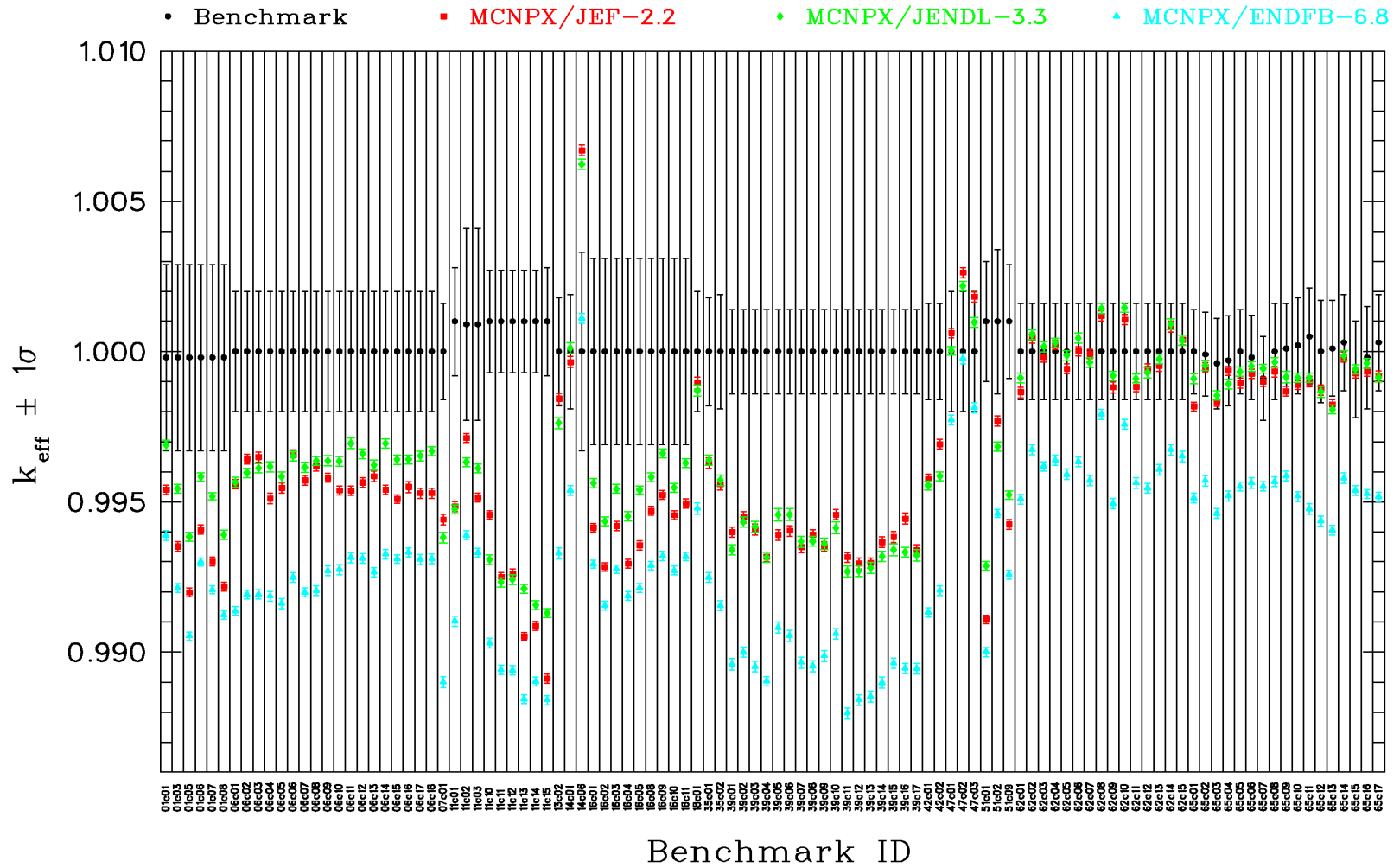
## 3. Results and Statistical Analysis

### 3.1 Calculated $k_{\text{eff}}$ Eigenvalues

The values for  $k_{\text{eff}}^{\text{calc}}$  obtained with MCNPX-2.5.0 using the JEF-2.2, JENDL-3.3 and ENDF/B-6.8 libraries are shown in Fig.1 in comparison to the  $k_{\text{eff}}^{\text{bench}}$  values of the 106 benchmark experiments, which are specified on the abscissa (the label 01c03, e.g., stands for LCT-001, case 03). The error bars represent the uncertainties which match one standard deviation with respect to the calculations. As 20 million active neutron histories were used, the MCNPX standard deviations  $\langle\sigma^{\text{MC}}\rangle$  are rather small (in the range of 10 to 20 pcm). As for most of the ICSBEP evaluations no confidence level for the benchmark uncertainties is given, we assumed it to be one standard deviation (like in the cases where the confidence level was explicitly specified).

The  $k_{\text{eff}}^{\text{calc}}$  values for case LCT-014-06 are relatively high in comparison to the other cases. This is in agreement with the results of the previous analysis [6] and the sample calculations performed with different codes and libraries that are presented in the benchmark specifications [6]. Grubb’s test [9] suggests (at the 5% confidence level) that the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  ratios obtained for LCT-014-06 (with all three libraries) are statistical outliers among the data sample, and we therefore dropped LCT-014-06 from the set of evaluated benchmarks.

**Figure 1:** Calculated and benchmark  $k_{eff}$  values with error bars representing one standard deviation



The following formulas were applied for the analysis of the  $k_{eff}^{calc}/k_{eff}^{bench}$  sample:

$$\left\langle \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right\rangle = \frac{1}{w} \sum_{n=1}^N w_n \left( \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right)_n ; \quad \sigma' = \frac{1}{\sqrt{w}} ; \quad w = \sum_{n=1}^N w_n ; \quad w_n = \frac{1}{\sigma_n^2} \quad (1)$$

$$\sigma_n = \left( \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right)_n \sqrt{\left( \frac{\sigma^{bench}}{k_{eff}^{bench}} \right)_n^2 + \left( \frac{\sigma^{calc}}{k_{eff}^{calc}} \right)_n^2} ; \quad s = \sqrt{\frac{1}{(N-3)} \sum_{n=1}^N \left( \left( \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right)_n - \left\langle \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right\rangle \right)^2} \quad (2)$$

Eqs. 1 and 2 give, respectively, the weighted average  $\langle k_{eff}^{calc}/k_{eff}^{bench} \rangle$  value and its standard deviation  $\sigma'$ , the uncertainty of a single observation  $\sigma_n$ , and the sample standard deviation  $s$ .

We will use  $s$  later on to evaluate the LTB based on the assumption of normality of the  $k_{eff}^{calc}/k_{eff}^{bench}$  population. Therefore we applied Eq.(2), which gives the best estimate of the standard deviation when a Gaussian distribution is assumed (see ICSBEP Guide to the Expression of Uncertainties from Ref. [6]). The results obtained are presented in Tab. 1.

**Table 1:** Statistical description of the calculated results.

MCNPX-version /Library	$\left\langle \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right\rangle \pm \sigma'$	Min $\left( \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right) \pm \sigma$	Max $\left( \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right) \pm \sigma$	Sample standard deviation, $s$	Size of sample, N
2.5.0/JEF-2.2	0.9964±0.0002	0.9881±0.0018	1.0026±0.0020	0.0031	105
2.5.0/JENDL-3.3	0.9966±0.0002	0.9903±0.0018	1.0022±0.0020	0.0028	105
2.5.0/ENDF/B-6.8	0.9928±0.0002	0.9874±0.0018	0.9998±0.0020	0.0028	105
2.4.0/JEF-2.2	0.9981±0.0002	0.9908±0.0018	1.0038±0.0020	0.0029	105
2.4.0/JENDL-3.3	0.9975±0.0002	0.9916±0.0018	1.0029±0.0020	0.0028	105

### 3.1.1 Comparison of Libraries

In the upper part of Tab.1 we compare the results calculated with MCNPX 2.5.0 using the JEF-2.2, JENDL-3.3 and ENDF/B-6.8 libraries. We find that JEF-2.2, JENDL-3.3 lead essentially to the same mean  $\langle k_{eff}^{calc}/k_{eff}^{bench} \rangle$  value: however the spread (between minimum and maximum) of the  $k_{eff}^{calc}/k_{eff}^{bench}$  distribution is slightly smaller, when the JENDL-3.3 library is applied. Although  $\langle k_{eff}^{calc}/k_{eff}^{bench} \rangle$  is slightly smaller than 1.0, the agreement with the benchmark cases is quite satisfactory. In contrast, the result for  $\langle k_{eff}^{calc}/k_{eff}^{bench} \rangle$  obtained with ENDF/B-6.8 is approximately 370 pcm smaller than for the other libraries and underestimates the benchmark cases on the average by 720 pcm.

### 3.1.2 MCNPX-2.5.0 versus MCNPX-2.4.0

In the lower part of Tab.1 the results of the previous analysis [6] are listed that were obtained with MCNPX-2.4.0 using the JEF-2.2 and JENDL-3.3 libraries. Notably, there are non-negligible differences between the results of these two versions of MCNPX, 170 pcm and 90 pcm, respectively, for the JEF-2.2 and JENDL-3.3 libraries. The differences were found to originate from an improved  $S(\alpha,\beta)$  thermal neutron scattering treatment in MCNPX-2.5.0 that removed nonphysical spikes in the thermal neutron spectrum [10].

### 3.2 Analysis of Trends with Respect to Experimental Design Parameters

Several relationships between the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  ratios and experimental benchmark design parameters were investigated. Tab. 2 gives the corresponding ranges that were covered. No statistically significant trends could be found for the parameters fuel enrichment, moderation ratio, fuel rod pitch size, and fuel pellet diameter.

**Table 2:** Ranges covered by the experimental benchmark design parameters.

Experimental design parameter	No trends found in the range	
	Minimum	Maximum
Fuel enrichment	2.35%	7.00%
Moderation ratio	1.50	3.00
Fuel rod pitch size	1.26 cm	2.29 cm
Fuel pellet diameter	0.743 cm	1.265 cm

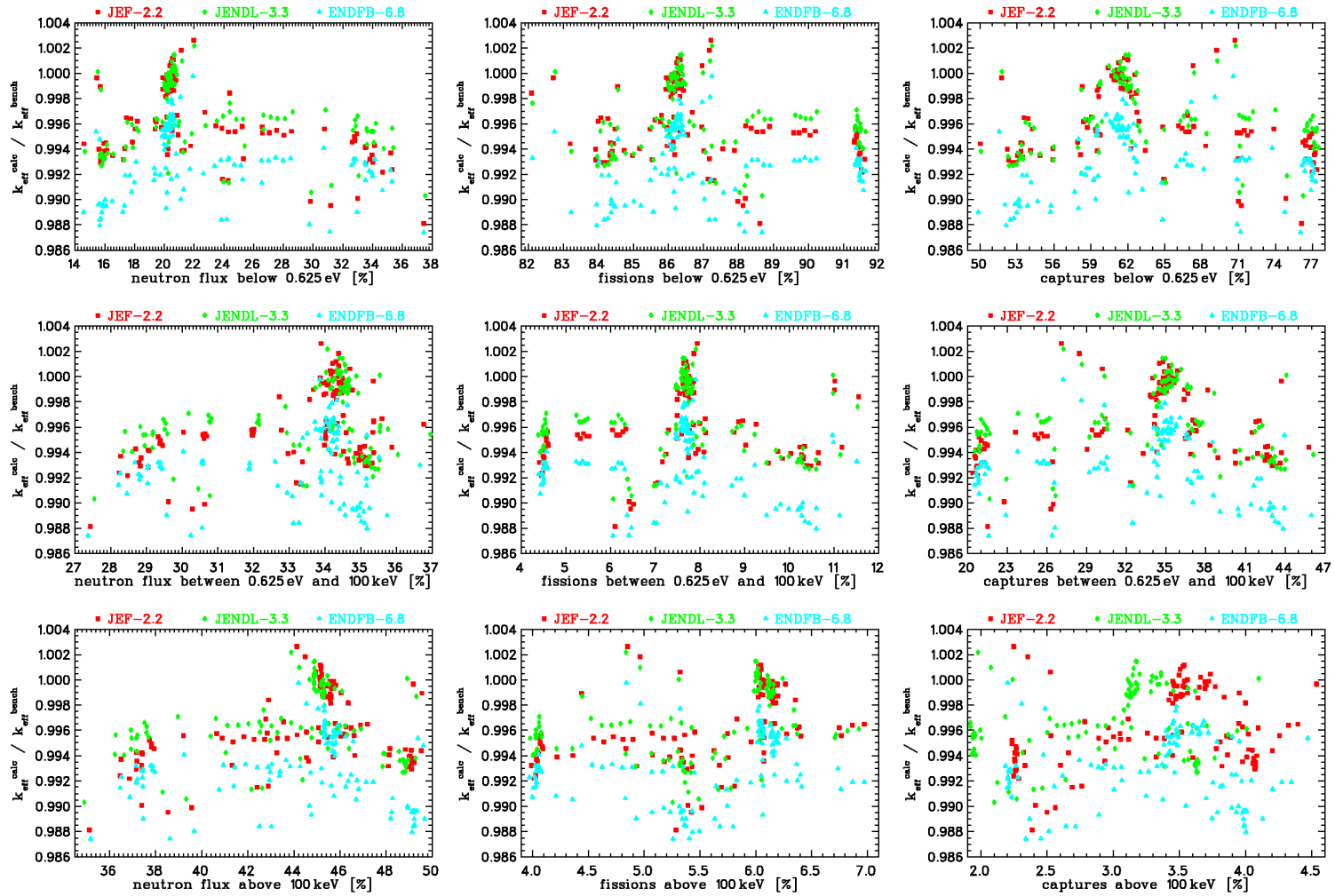
### 3.3 Analysis of Calculated Spectrum-related Characteristics

In order to assess the range of applicability of MCNPX-2.5.0 in combination with the three libraries and to get indications of possible deficiencies that would cause the calculations to underestimate the benchmark  $k_{\text{eff}}$  eigenvalues, we have studied spectrum-related trends in the criticality calculation results. Following Ref.[5] these include: the energy corresponding to the average neutron lethargy causing fission (EALF), the average neutron energy causing fission (AFGE), the neutron gas temperature in the thermal energy range ( $T_n$ ), the percentage of the neutron flux, fissions, and captures that occur in a three- (thermal, intermediate, fast) and thirty-group energy mesh, the percentage of fissions (of  $^{235}\text{U}$ ,  $^{238}\text{U}$ ) and captures by isotopes ( $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{16}\text{O}$ ,  $^1\text{H}$ ,  $^{27}\text{Al}$ ) over the core region, and the number of average fission neutrons produced per neutron absorbed in the core ( $\nu\Sigma_f/\Sigma_a$ ). No statistically significant trends could be identified for any of these parameters. A typical outcome of the spectrum-related trend analysis is shown in Fig. 2.

In the diagrams of the upper, middle, and lower rows, respectively, the ratio  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  for the 105 benchmarks is plotted versus the percentage of neutron flux (first column), fissions (second column), and captures (third column) that occur in the thermal (neutron energy  $E_n < 0.625$  eV), intermediate ( $0.625 < E_n < 100$  keV), and fast ( $E_n > 100$  keV) energy ranges. Within each diagram the results obtained with the three libraries are compared. Linear fits (not shown in the diagrams) have been performed, and the corresponding errors in the slope and confidence levels were determined. The uncertainty of the slopes of most of the trends was found to be quite large, and the corresponding confidence level was zero. In those few cases where the error of the slope was relatively small (i.e. between 10 and 20%) the confidence levels of the linear fits amounted to less than 1%. Thus, no evidence for statistically significant trends was found which would have to be included in future determinations of an upper subcriticality limit (USL).

Tabs. 3 and 4 provide quantitative indication of the range of applicability of the lower tolerance bounds estimated below. The energy ranges for the considered reactions, as calculated with the three different libraries, are generally found to be very similar, except for captures in  $^{16}\text{O}$ . Here the range calculated with the JENDL-3.3 library does not overlap with

**Figure 2:**  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  ratios versus neutron flux (1st column), fissions (2nd column), and captures (3rd column) in the thermal, intermediate and fast energy range obtained with three libraries.



**Table 3:** Range of percentages of the neutron flux, fissions and captures in a thirty-group energy mesh.

E <sub>upper</sub> , (eV)	neutron flux						fissions						captures					
	JEF-2.2		JENDL-3.3		ENDF/B-6.8		JEF-2.2		JENDL-3.3		ENDF/B-6.8		JEF-2.2		JENDL-3.3		ENDF/B-6.8	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
1.000E-02	0.42	1.85	0.41	1.79	0.41	1.78	5.41	9.01	5.33	8.95	5.34	8.94	4.15	9.40	4.08	9.17	4.06	9.15
2.154E-02	1.13	4.56	1.14	4.55	1.13	4.54	11.25	16.38	11.40	16.52	11.41	16.52	7.21	14.21	7.34	14.36	7.29	14.31
4.642E-02	3.03	10.78	3.02	10.72	3.00	10.70	23.20	29.61	23.24	29.58	23.27	29.59	13.73	24.23	13.61	24.17	13.55	24.09
1.000E-01	4.46	12.59	4.46	12.71	4.43	12.68	24.02	26.09	23.95	26.12	23.94	26.11	14.20	21.28	14.11	21.38	14.05	21.33
2.154E-01	2.93	5.18	2.96	5.23	2.94	5.22	7.93	11.01	7.83	10.90	7.84	10.90	6.38	9.46	6.46	9.54	6.44	9.50
4.642E-01	1.83	2.21	1.88	2.26	1.87	2.24	2.55	5.51	2.57	5.55	2.57	5.54	1.83	4.47	1.91	4.61	1.90	4.60
1.000E+00	1.66	2.11	1.69	2.15	1.68	2.13	0.96	2.37	0.97	2.39	0.98	2.39	0.97	3.06	0.98	3.11	0.98	3.10
2.154E+00	1.56	2.01	1.59	2.05	1.58	2.03	0.50	1.25	0.50	1.27	0.51	1.27	0.77	2.43	0.78	2.45	0.78	2.45
4.642E+00	1.51	1.96	1.53	1.99	1.53	1.98	0.23	0.58	0.24	0.61	0.24	0.61	0.67	2.27	0.68	2.31	0.68	2.30
1.000E+01	1.39	1.77	1.39	1.78	1.39	1.76	0.53	1.23	0.52	1.22	0.52	1.21	5.13	10.99	5.16	10.98	5.13	10.95
2.154E+01	1.49	1.95	1.49	1.95	1.48	1.94	0.56	1.35	0.54	1.32	0.54	1.32	2.80	6.38	2.83	6.42	2.81	6.39
4.642E+01	1.40	1.86	1.40	1.86	1.40	1.85	0.51	1.31	0.50	1.29	0.50	1.29	2.52	5.76	2.54	5.85	2.54	5.82
1.000E+02	1.74	2.34	1.74	2.35	1.73	2.33	0.51	1.41	0.51	1.40	0.51	1.39	1.41	3.50	1.44	3.58	1.43	3.54
2.154E+02	1.64	2.22	1.64	2.22	1.63	2.21	0.28	0.81	0.28	0.80	0.28	0.79	1.67	3.92	1.69	4.02	1.69	3.99
4.642E+02	1.69	2.30	1.69	2.30	1.68	2.29	0.24	0.70	0.24	0.71	0.24	0.71	0.97	2.32	0.99	2.40	0.99	2.39
1.000E+03	1.71	2.34	1.72	2.34	1.71	2.33	0.17	0.50	0.17	0.50	0.17	0.50	0.92	2.18	0.93	2.22	0.93	2.20
2.154E+03	1.75	2.39	1.75	2.40	1.74	2.39	0.11	0.33	0.11	0.33	0.11	0.33	0.74	1.77	0.74	1.78	0.74	1.78
4.642E+03	1.80	2.47	1.80	2.47	1.79	2.46	0.08	0.24	0.08	0.23	0.08	0.24	0.60	1.45	0.60	1.46	0.60	1.46
1.000E+04	1.86	2.57	1.86	2.58	1.85	2.56	0.06	0.17	0.05	0.17	0.06	0.17	0.53	1.31	0.52	1.30	0.52	1.29
2.154E+04	1.98	2.76	1.98	2.76	1.97	2.74	0.05	0.14	0.04	0.14	0.05	0.14	0.47	1.23	0.44	1.13	0.47	1.22
4.642E+04	2.21	3.09	2.23	3.11	2.20	3.08	0.04	0.13	0.04	0.12	0.04	0.13	0.37	1.00	0.37	0.98	0.38	1.00
1.000E+05	2.68	3.83	2.70	3.86	2.67	3.77	0.04	0.13	0.04	0.13	0.04	0.13	0.26	0.72	0.27	0.73	0.26	0.71
2.000E+05	3.21	4.70	3.23	4.74	3.19	4.63	0.04	0.14	0.04	0.14	0.04	0.13	0.20	0.55	0.20	0.56	0.20	0.54
4.000E+05	4.60	6.62	4.64	6.72	4.61	6.66	0.06	0.18	0.06	0.18	0.06	0.18	0.23	0.63	0.24	0.64	0.23	0.62
8.000E+05	6.44	9.20	6.43	9.20	6.52	9.35	0.08	0.23	0.08	0.23	0.08	0.23	0.32	0.82	0.33	0.84	0.33	0.84
1.400E+06	6.04	8.72	6.01	8.70	6.15	8.85	0.18	0.37	0.18	0.38	0.18	0.38	0.30	0.73	0.31	0.74	0.31	0.75
2.500E+06	7.18	10.35	7.09	10.28	7.21	10.39	1.60	2.79	1.59	2.76	1.61	2.83	0.18	0.41	0.19	0.43	0.18	0.41
4.000E+06	4.75	6.90	4.64	6.76	4.70	6.85	1.19	2.04	1.19	2.02	1.19	2.03	0.08	0.17	0.05	0.13	0.09	0.17
6.500E+06	2.37	3.36	2.33	3.30	2.30	3.29	0.61	1.04	0.60	1.03	0.60	1.01	0.58	0.92	0.37	0.57	0.56	0.89
2.000E+07	0.50	0.70	0.49	0.69	0.48	0.68	0.21	0.36	0.21	0.35	0.20	0.34	0.24	0.39	0.17	0.27	0.21	0.33

the ranges obtained with JEF-2.2 and ENDF/B-6.8. Clearly, no significant effect on the calculated  $k_{eff}$  -eigenvalues is expected, but the cause of significantly less captures in  $^{16}\text{O}$  using JENDL-3.3 should be clarified.

**Table 4:** Ranges for spectrum-related observables that were covered by the calculations applying the JEF-2.2, JENDL-3.3, and ENDF/B-6.8 libraries.

Library	JEF-2.2	JENDL-3.3	ENDF/B-6.8
Observable	No Trends found in the range		
	Minimum – Maximum		
EALF	0.096 – 0.304 eV	0.096 – 0.302 eV	0.096 – 0.303 eV
AFGE	0.269 – 0.653 eV	0.268 – 0.649 eV	0.268 – 0.651 eV
$T_n$	356 – 522 K	360 – 526 K	360 – 526 K
Fissions $^{235}\text{U}$	43.4 – 63.6 %	43.5 – 63.6 %	43.4 – 63.5 %
Fissions $^{238}\text{U}$	1.81 – 3.38 %	1.80 – 3.35 %	1.80 – 3.37 %
Captures $^{235}\text{U}$	8.29 – 12.9 %	8.43 – 13.2 %	8.40 – 13.2 %
Captures $^{238}\text{U}$	14.4 – 25.6 %	14.4 – 25.5 %	14.4 – 25.5 %
Captures $^{16}\text{O}$	0.447 – 0.509 %	0.281 – 0.317 %	0.415 – 0.469 %
Captures $^1\text{H}$	4.96 – 26.2 %	4.95 – 26.0 %	4.94 – 26.1 %
Captures $^{27}\text{Al}$	0.024 – 0.877 %	0.025 – 0.928 %	0.026 – 0.951 %
$\nu\Sigma_f/\Sigma_a$	1.115 – 1.552	1.115 – 1.550	1.112 – 1.548

### 3.4 Estimation of a Lower Tolerance Bound for $k_{eff}$

#### 3.4.1 Analysis Based on the Assumption of Normality

Following Ref.[11] the one-sided statistical LTB to be exceeded by at least a proportion  $p$  of the normally distributed  $k_{eff}^{calc}/k_{eff}^{bench}$  population is given by the expression:

$$K_{eff}^{LTB} = \left\langle \frac{k_{eff}^{calc}}{k_{eff}^{bench}} \right\rangle - k_1(\alpha, p, N) \cdot s \quad (3)$$

where the coverage factor  $k_1$  depends on the confidence level  $\alpha$ , the proportion of the population  $p$ , and the sample size  $N$ . The factor  $k_1$  can be extracted from statistical tabulations [11]. In Tab.5 the LTBs calculated accordingly are listed for different values of the proportion  $p$  and the confidence level  $\alpha$ .



**Table 5:** One-sided statistical tolerance bounds to contain the specified proportion of a normally distributed  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  population with a confidence level  $\alpha$ .

Proportion $p$ :	90%	95%	95%	99%	99.5%
Confidence Level $\alpha$ :	90%	95%	99.5%	99%	99.5%
Coverage factor $k_1$	1.46	1.92	2.10	2.84	3.20
2.5.0/JEF-2.2	0.9919	0.9905	0.9899	0.9876	0.9865
2.5.0/JENDL-3.3	0.9925	0.9912	0.9907	0.9887	0.9876
2.5.0/ENDF/B-6.8	0.9887	0.9874	0.9869	0.9849	0.9838
2.4.0/JEF-2.2	0.9939	0.9926	0.9921	0.9899	0.9889
2.4.0/JENDL-3.3	0.9935	0.9922	0.9917	0.9897	0.9887

3.4.2 Analysis Based on the Distribution-free Approach

Using order statistics, the one-sided statistical LTB for the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  population is determined as endpoint  $(k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}})_l$  of the ordered sample with size  $N$ , and  $L$  chosen as the largest integer such that [11]:

$$1 - \sum_{i=0}^{L-1} \frac{N!}{i!(N-i)!} p^i (1-p)^{N-i} \geq 1 - \alpha \tag{4}$$

The LTBs determined according to Eq.(4) are listed in Tab. 6 for different values of the proportion  $p$  and the confidence level  $\alpha$ , that can be evaluated based on 105 observations.

**Table 6:** One-sided statistical tolerance bounds to contain the specified proportion of a  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  population with a confidence level  $\alpha$  based on order statistics.

Proportion $p$ :	90%	95%	95%
Confidence Level $\alpha$ :	91%	97%	99.5%
$L$	7	2	1
2.5.0/JEF-2.2	0.9922	0.9895	0.9881
2.5.0/JENDL-3.3	0.9921	0.9906	0.9903
2.5.0/ENDF/B-6.8	0.9884	0.9874	0.9874
2.4.0/JEF-2.2	0.9939	0.9918	0.9908
2.4.0/JENDL-3.3	0.9933	0.9918	0.9916

4. Discussion and Conclusions

A set of three continuous-energy neutron data libraries using the Monte Carlo radiation transport code MCNPX has been assessed for light water reactor criticality safety applications by comparison with a suite of low-enriched thermal compound uranium benchmarks. The calculated  $k_{\text{eff}}$ -values were found to be in good agreement with the reference benchmark values (within  $\pm 2\sigma$ ), although the weighted average  $\langle k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}} \rangle$  of all benchmarks underestimates criticality by 360 pcm, 340 pcm, and 720 pcm using the JEF-2.2, JENDL-3.3, and ENDF/B-6.8 libraries, respectively. These results confirm the long-standing problem of low eigenvalues in water-reflected low-enriched-uranium fuel lattice systems [12]. An improved  $S(\alpha, \beta)$  thermal neutron scattering treatment implemented in MCNPX-2.5.0 did not mitigate this problem.

Analysis of spectrum-related trends in  $k_{\text{eff}}$  and trends related to experimental design parameters has been performed and thereby the range of applicability of the reported estimates of lower tolerance bounds has been well explored. Statistically significant trends could not be found. One consequence of this finding is that there is no need to include trends in future determinations of an upper subcriticality limit (USL) using MCNPX and the specified libraries. MCNPX appears to be a reliable tool to analyze a rather wide range of critical configurations. Furthermore, due to the absence of trends, it is expected that moderate extrapolations outside the range of validation of the sets of Monte-Carlo Code/cross section libraries may be well justifiable. The second consequence is that the underestimation of the benchmark eigenvalues remains unexplained.

In addition, we also confirmed the findings from the previous analysis [6] that the differences between LTBs derived based on a distribution-free approach and LTBs estimated based on the assumption of normality of the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  population turn out to be minor for all libraries (less than 200 pcm: compare the results in Tables 5 and 6). This lends support to the usual practice of basing criticality safety evaluations on the assumption of normality of the  $k_{\text{eff}}^{\text{calc}}/k_{\text{eff}}^{\text{bench}}$  distribution as this approach is very convenient for practical applications, especially if the number of available benchmark experiments is relatively small.

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