Validation of KENO V.a Using ENDF/B-VI and ENDF/B-VII for Criticality Safety Applications

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Abstract

An upper subcritical limit (USL), which includes allowance for bias and bias uncertainty in the calculated k_{eff}, needs to be established for all criticality safety code calculations. In this paper, the bias and bias uncertainty associated with k_{eff} values computed using KENO V.a are evaluated based on benchmark experiments for ^{235}U, ^{233}U, ^{239}Pu and MOX systems. The code validation is performed using the 238-group ENDF/B-VI and ENDF/B-VII cross-section libraries provided in the SCALE code package [1]. The evaluation suggests that the ENDF/B-VII library performs better than the ENDF/B-VI, with biases less than 2 mk for most systems.

1. Introduction

Establishing an Upper Subcritical Limit (USL) for the calculation of the effective neutron multiplication factor (k_{eff}) is required by CNSC regulations for all criticality safety calculations using a computer code [2]. In criticality safety, the USL is the maximum allowed value of the calculated k_{eff}, established to ensure that under normal and credible abnormal conditions, the systems assessed to be subcritical will actually be subcritical. Aside from an administrative margin of subcriticality of 50 mk, the USL must also allow for both the bias in the calculation of k_{eff}, and the uncertainty in the bias. Hence, validation exercises based on benchmark experiments are needed to establish the code bias and bias uncertainty for fissile material systems of interest.

This paper summarizes two validation exercises, one performed using the 238-group ENDF/B-VI cross-section library distributed with the SCALE 5.1 code package [1] and one using the 238-group ENDF/B-VII cross-section library distributed with the SCALE 6.0 code package [1]. In a series of validation exercises, the bias and bias uncertainty associated with the calculation of k_{eff} using KENO V.a were determined for benchmark systems with pure ^{233}U and ^{239}Pu systems, ^{235}U in low-enriched uranium (LEU) and high-enriched uranium (HEU) systems and mixed ^{239}Pu and natural uranium (MOX) systems. The analysis included both fast and thermal systems for each type of material, and, when available, intermediate-energy and mixed-spectrum systems. Also, a range of geometries, moderators and reflectors were considered when choosing the subset of benchmark experiments from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (IHECSBE) [3].

Throughout this validation study, the bias refers to the difference between the overall calculated k_{eff} value for a set of experiments and a k_{eff} value of 1.000, corresponding to a critical system. The uncertainty associated with the calculated k_{eff} value accounted for the Monte Carlo standard deviation of the calculated k_{eff}, and the benchmark uncertainty reported in the IHECSBE [3], which includes uncertainties in the critical experiment and uncertainties due to limitations in the geometrical or material representations used in the computational mode. For each type of fissile material system investigated in this paper, the average bias and estimated bias uncertainty for a set of experiments was reported and compared for the two cross-section libraries. These values can be used in establishing the USL for a particular system.

2. General Description and Methodology

2.1 Computer Code Package

KENO V.a [1], a functional module within the SCALE suite of codes, is a multigroup Monte Carlo criticality code used to calculate k_{eff} of an assembly including fissionable materials. Validation of KENO V.a is performed using the 238-group ENDF/B-VI cross-section library for the version provided in the SCALE 5.1 package, and using the 238-group ENDF/B-VII cross-section library for the version provided in the SCALE 6.0 package. CENTRM (Continuous ENergy TRansport Module) was used to obtain the problem-dependent neutron spectra for processing self-shielded multigroup cross-sections. CENTRM is the module that is strongly recommended by the code authors to be used with the 238-group ENDF/B-VI or ENDF/B-VII libraries in SCALE 5.1 or 6.0.

Some models (e.g., Pu systems using the ENDF/B-VI cross-section library) were run on a Windows platform. However, most models, including all those using the ENDF/B-VII cross-section library, were run on a Linux platform[1].

2.2 Validation Models

Criticality safety benchmark experiments were selected from the IHECSBE [3] for each type of system. Table 1 summarizes the types of systems chosen for the validation exercise, which included fissile nuclides such as ^{235}U, ^{233}U, and ^{239}Pu. The experiments also covered a range of moderators (e.g. light water, heavy water, polyethylene and polystyrene), reflectors (e.g. lead, natural uranium, plexiglass, light water, graphite, beryllium and thorium), geometries, fuel pin arrangements, lattice pitches, and enrichments. Experiments with both fast and thermal systems were included, along with a number of systems having mixed fast, intermediate and thermal spectra. Mixed oxide (MOX) systems were also modelled, with PuO_2 in MOX concentrations of 2 wt%, 6.6 wt% and 20 wt%.

[1] The installation of KENO V.a has been verified against an extensive set of test cases on both platforms, so these validation results may be applied to KENO V.a calculations of k_{eff} on either system.

Table 1 Summary of Benchmark Experiments Used to Validate KENO V.a

System Type	Number of Benchmark Experiments	Energy Spectrum	Physical Form	Moderators	Reflectors
HEU[2]	20	Fast	Metal	Be, BeO_2, polyethylene, H_2O, D_2O	H_2O, D_2O, polyethylene, lead, natural/depleted uranium, Be, graphite, concrete, plexiglass
	2	Thermal	Metal		
	41	Thermal	Solution		
LEU[3]	13	Thermal	Metal	H_2O, D_2O	H_2O
	13	Thermal	Compound		
	12	Thermal	Solution		
^{233}U	7	Fast	Metal	H_2O	H_2O, HEU, Be, paraffin
	31	Thermal	Solution		
^{239}Pu	5	Fast	Metal	Polystyrene, H_2O	Thorium, natural uranium, H_2O, plexiglass
	19	Thermal	Solution		
	29	Mixed	Compound		
MOX	16	Thermal	Compound	H_2O	H_2O

2.3 Methods

The KENO V.a models of the experiments were based on the description provided in the IHECSBE [3]. The models were run using 1500 neutrons per generation for a maximum of 2000 generations, or until a standard deviation ≤1.0 mk in the final estimate of k_{eff} was achieved.

To assess the general performance of each cross-section library, the calculated k_{eff} values were compared to the benchmark k_{eff} values. Although the experiments are critical experiments, (i.e., the experimental k_{eff} value is 1.000), simplifications are sometimes necessary in the benchmark model specifications. The effect of these simplifications on k_{eff} was carefully quantified (either from measurement or from calculations) in the benchmark description provided in the IHECSBE [3], which resulted in an adjusted experimental k_{eff} value that was referred to as the benchmark k_{eff} value. The models used in this paper make the same assumptions and simplifications as those described in the IHECSBE [3].

The overall calculated k_{eff} value for each type of system was obtained from the individual calculated k_{eff} values for a subset of experiments, as follows:

$$k_c = 1 + \frac{\sum \frac{k_{ci} - k_{Bi}}{\sigma_{ki}^2}}{\sum \frac{1}{\sigma_{ki}^2}}, \qquad (1)$$

[2] High-Enriched Uranium (HEU) is defined as uranium with >20 wt% ^{235}U in U.
[3] Low-Enriched Uranium (LEU) is defined as uranium with ≤ 20 wt% ^{235}U in U.

where k_c is the calculated k_{eff} value for the entire set of benchmark experiments, k_{ci} is the calculated k_{eff} value for the ith benchmark experiment in the set, k_{Bi} is the benchmark k_{eff} value for the ith benchmark experiment obtained from the IHECSBE [3], and σ_{ki} is the combined benchmark uncertainty obtained from the IHECSBE [3] disk, which accounts for uncertainties in material compositions, geometry and model specifications, and Monte Carlo standard deviation for the ith benchmark experiment.

The bias is identified by subtracting the k_{eff} value corresponding to a critical system (i.e., 1.000) from the k_c value calculated using equation (1). The uncertainty which applies to this bias is the same as the overall uncertainty associated with the value of k_c, which was calculated as follows:

$$\Delta k_c = \sqrt{\frac{\sum \frac{(k_{ci} - k_c)^2}{\sigma_{ki}^2}}{N \times \sum \frac{1}{\sigma_{ki}^2}}}, \tag{2}$$

where N is the number of independent experiments in the set. In the absence of clear information regarding the correlations between experiments in a chosen subset, a conservative approach was adopted by setting N=1.

3. Validation Results

3.1 High-Enriched Uranium Systems

A total of 63 critical experiments were modelled using both ENDF/B-VI and ENDF/B-VII 238-group cross-section libraries. Overall bias and bias uncertainties values were determined for thermal and fast systems separately, as well as for the entire subset of HEU experiments. Using the ENDF/B-VI cross-section library, the $k_c \pm \Delta k_c$ values are 0.9961 ± 0.0052 and 0.9974 ± 0.0064 for the fast and thermal systems respectively. The use of the ENDF/B-VII cross-section library resulted in $k_c \pm \Delta k_c$ values of 0.9996 ± 0.0036 and 0.9977 ± 0.0073 for the fast and thermal systems respectively.

A direct comparison between the calculated k_{eff} values and the benchmark k_{eff} values is illustrated in Figure 1 for the fast systems and in Figure 2 for the thermal systems. The error bars indicate the effective uncertainties in the benchmark k_{eff} values, as reported in the IHECSBE [3].

The combined trend from Figure 1 and Figure 2 results in an overall smaller negative bias when ENDF/B-VII was used, that is, the $k_c \pm \Delta k_c$ obtained using ENDF/B-VII is 0.9991 ± 0.0046, while that obtained using ENDF/B-VII is 0.9965 ± 0.0056.

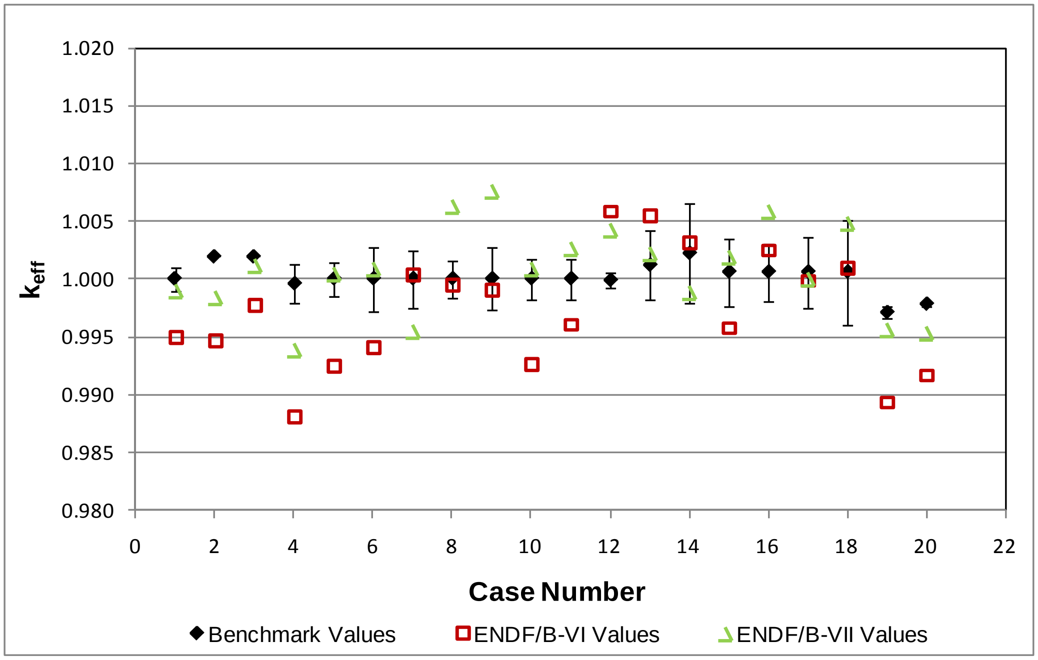

Figure 1 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for HEU fast systems.

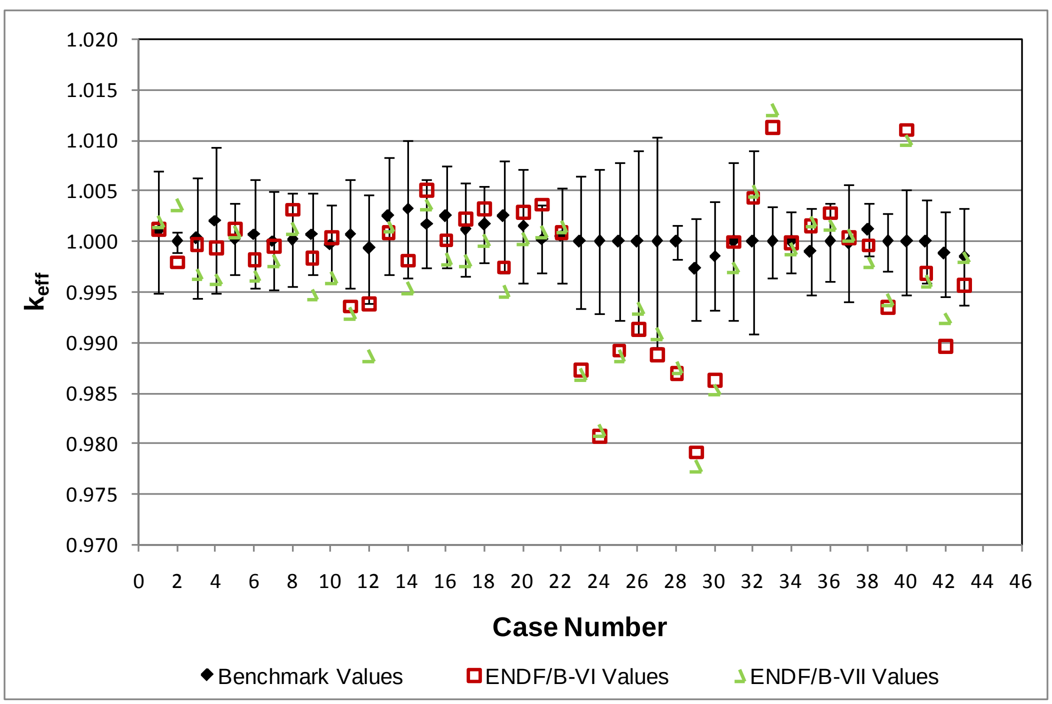

Figure 2 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for HEU thermal systems.

3.2 Low-Enriched Uranium Systems

To determine the bias and bias uncertainty for LEU systems, 38 critical experiments were modelled using the ENDF/B-VI and ENDF/B-VII cross-section libraries. All experiments were thermal systems, of which 26 were light water moderated and 12 were heavy water moderated. The $k_c \pm \Delta k_c$ values determined using the ENDF/B-VI cross-section library are 0.9944 ± 0.0045 and 1.0001 ± 0.0086 for light water and heavy water moderated systems respectively. The use of the ENDF/B-VII cross-section library resulted in $k_c \pm \Delta k_c$ values of 0.9984 ± 0.0036 and 1.0042 ± 0.0091 for light water and heavy water moderated systems respectively.

A direct comparison between the calculated k_{eff} values and the benchmark k_{eff} values is illustrated in Figure 3. The error bars indicate the effective uncertainties in the benchmark k_{eff} values, as reported in the IHECSBE [3]. The results using the ENDF/B-VII library showed a positive shift in the bias for both light water moderated systems (cases 1 to 26) and heavy water moderated systems (cases 27 to 38). Furthermore, the use of the ENDF/B-VII library resulted in a lower bias for the light water moderated cases relative to the heavy water moderated ones. In terms of overall bias, the use of the ENDF/B-VII library ($k_c \pm \Delta k_c$ of 0.9985 ± 0.0038) resulted in a smaller negative bias than that of the ENDF/B-VI library ($k_c \pm \Delta k_c$ of 0.9946 ± 0.0047).

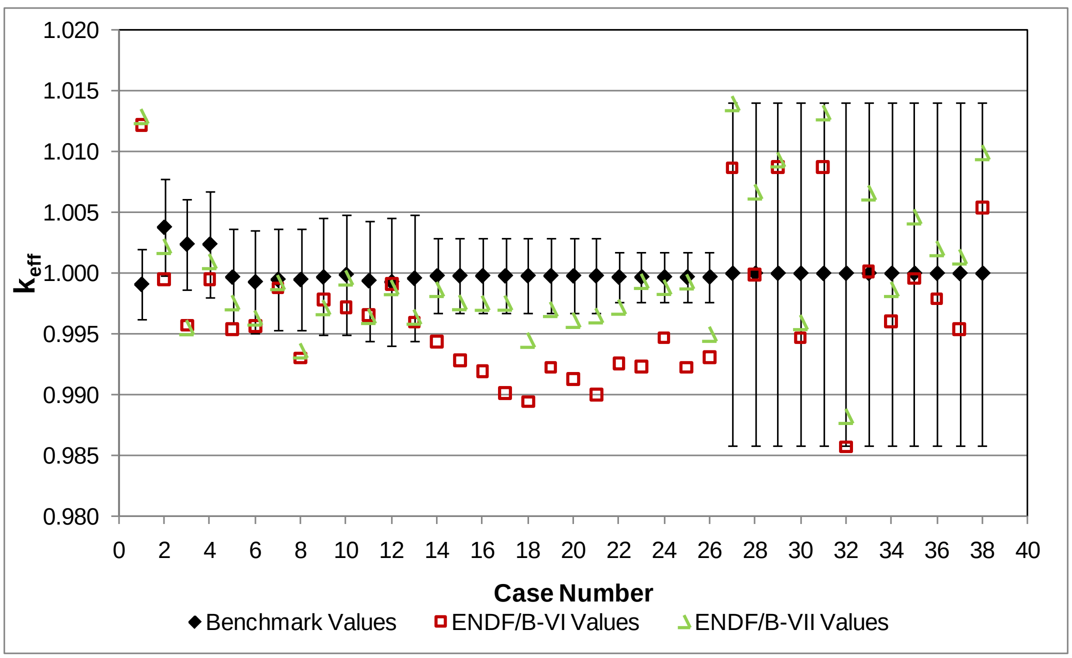

Figure 3 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for LEU thermal systems.

3.3

^{233}U Systems

A total of 38 cases were modelled for ^{233}U systems. Cases 1 to 7 are fast systems, while cases 8 to 38 are thermal systems. The results from the calculated k_{eff} values using both the ENDF/B-VI and ENDF/B-VII cross-section libraries were compared with the benchmark k_{eff} values in Figure 4. The error bars indicate the effective uncertainties in the benchmark k_{eff} values, as reported in the IHECSBE [3]. Note that cases 8 to 23 have higher uncertainties in the benchmark k_{eff} values, to account for neglecting impurities in the fissile solution and for geometry simplifications/uncertainties.

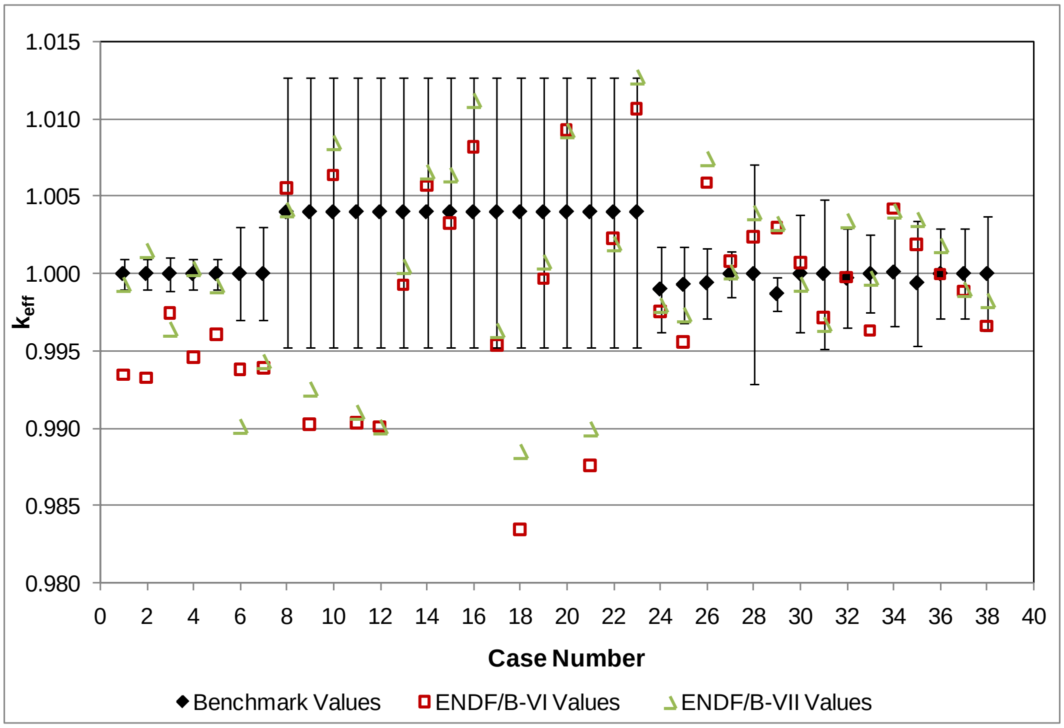

Figure 4 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for ^{233}U systems.

The average $k_c \pm \Delta k_c$ values for fast systems using the ENDF/B-VI and ENDF/B-VII library were 0.9949 ± 0.0030, and 0.9989 ± 0.0028 respectively. The $k_c \pm \Delta k_c$ values for thermal systems using the ENDF/B-VI and ENDF/B-VII libraries were 1.0005 ± 0.0049 and 1.0014 ± 0.0039 respectively. In general, a positive shift in the bias of k_{eff} was observed for both energy spectra, when the ENDF/B-VII library was used. The use of the ENDF/B-VI library resulted in an overall $k_c \pm \Delta k_c$ value of 0.9974 ± 0.0040, while that of the ENDF/B-VII library resulted in an overall $k_c \pm \Delta k_c$ value of 1.0000 ± 0.0033.

3.4 ^{239}Pu Systems

To determine the bias and bias uncertainty for ^{239}Pu systems, 53 critical experiments were modelled. A comparison between the calculated k_{eff} values and the benchmark k_{eff} values for fast and thermal systems is illustrated in Figure 5. The calculation results obtained for intermediate-spectra ^{239}Pu critical experiments are illustrated in Figure 6. The error bars in Figure 5 and Figure 6 indicate the effective uncertainties in the benchmark k_{eff} values, as reported in the IHECSBE [3]. Note that cases 6 to 24 have higher uncertainties in the benchmark k_{eff} values, to account for uncertainties in Pu solution density and composition and determination of the critical volume.

In general, for the fast systems (cases 1 to 5 in Figure 5), the use of the ENDF/B-VII library resulted in a smaller bias and bias uncertainty than that of the ENDF/B-VI library. The calculated $k_c \pm \Delta k_c$ values for fast systems were 1.0026 ± 0.0045 and 0.9983 ± 0.0016, for the ENDF/B-VI and ENDF/B-VII library respectively. For thermal systems (cases 6 to 24 in Figure 5), ENDF/B-VII library results in a smaller bias, but a larger bias uncertainty. The $k_c \pm \Delta k_c$ obtained for thermal systems were 1.0037 ± 0.0031 and 1.0032 ± 0.0055, for the ENDF/B-VI and ENDF/B-VII libraries respectively.

In comparison, for intermediate-energy systems (energies between 1 eV and 10 keV), both cross-section libraries resulted in large positive biases and bias uncertainties, which could indicate possible problems in the base ENDF/B-VI and ENDF/B-VII cross-section data for ^{239}Pu systems. Further studies are required to investigate the performance of the cross-section libraries for ^{239}Pu systems in the intermediate-energy range, and identify factors which could result in the large positive bias observed here. The overall $k_c \pm \Delta k_c$ for intermediate-energy systems was calculated at 1.0216 ± 0.0200 and 1.0246 ± 0.0258, for the ENDF/B-VI and ENDF/B-VII library respectively.

Since the intermediate-energy systems lead to an unrealistically large positive bias, it is advisable to not include these results in the calculation for the overall bias and bias uncertainty for pure ^{239}Pu systems. Hence, the overall calculated $k_c \pm \Delta k_c$, not including intermediate-energy systems, was 1.0028 ± 0.0042 and 0.9995 ± 0.0031, for the ENDF/B-VI and ENDF/B-VII libraries respectively.

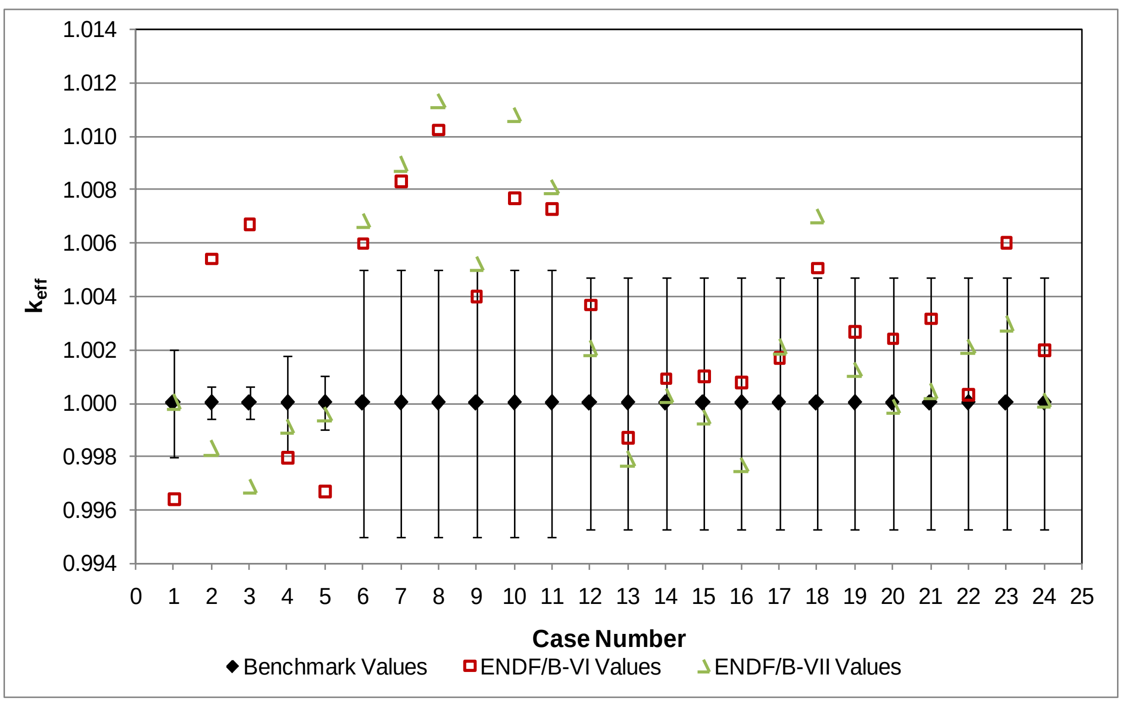

Figure 5 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for ^{239}Pu fast (cases 1 to 5) and thermal (cases 6 to 24) systems.

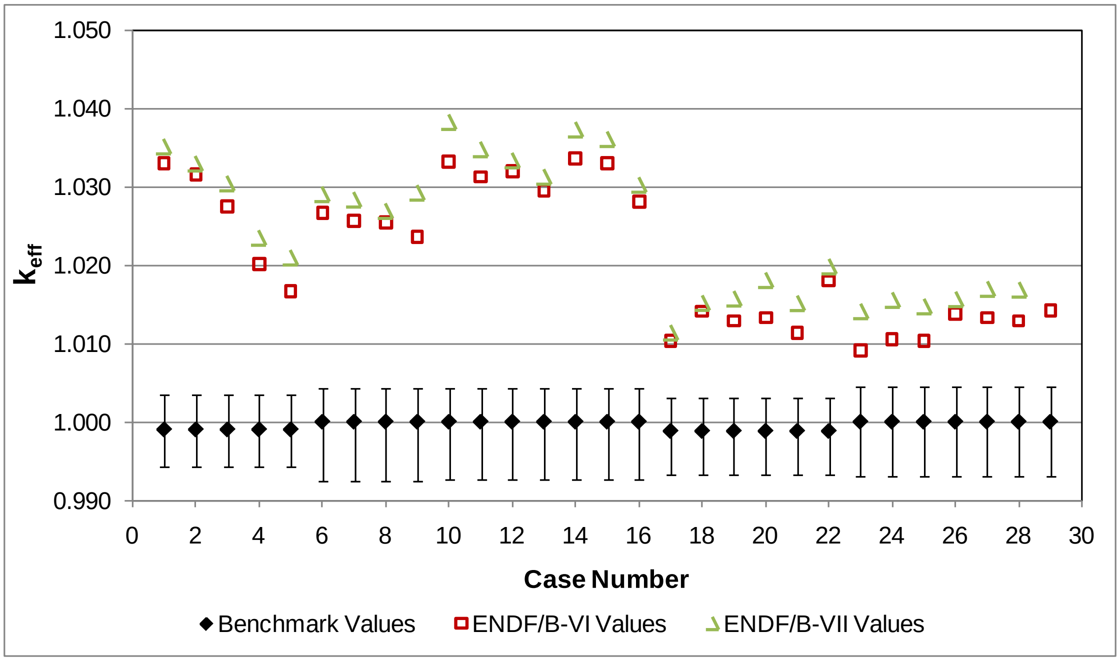

Figure 6 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for intermediate-energy ^{239}Pu systems.

3.5 MOX Systems

A total of 16 critical experiments were selected to determine the bias and bias uncertainty for MOX systems. The experiments are all light water moderated systems, with a maximum of 20 wt% Pu concentration in MOX. The most thermal systems (cases 1 to 10 in Figure 7, with energies <0.30 eV) resulted in k_{eff} value of approximately 1.000, while those with a harder spectrum (cases 11 to 16 in Figure 7, with energies between 0.30 eV and 1 eV) resulted in a slightly negative bias. The error bars in Figure 7 indicate the effective uncertainties in the benchmark k_{eff} values, as reported in the IHECSBE [3].

The overall calculated $k_c \pm \Delta k_c$ for the MOX systems was 0.9960 ± 0.0028 and 1.0007 ± 0.0030, for ENDF/B-VI and ENDF/B-VII libraries respectively. As illustrated also in Figure 7, using the ENDF/B-VI library resulted in a negative bias for almost all critical experiments modelled, while the ENDF/B-VII library resulted in an increase in the k_{eff} values, most of them leading to a positive bias.

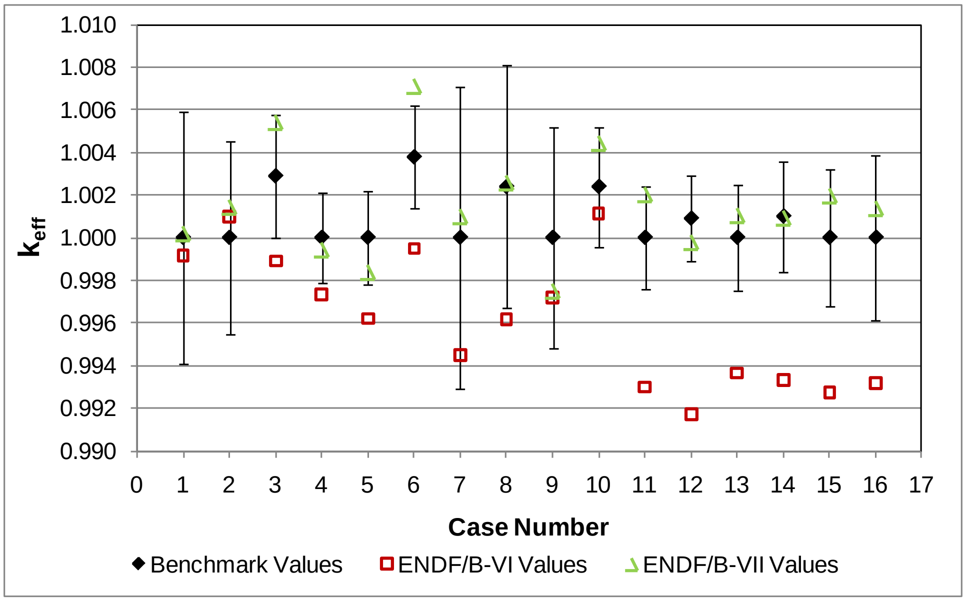

Figure 7 Comparison between the results using the 238-group ENDF/B-VI and ENDF/B-VII libraries and the benchmark k_{eff} values for MOX systems.

3.6 Summary of Bias and Bias Uncertainty Results and Discussion

The bias and bias uncertainty values for the calculation of k_{eff} were established in this paper for various fissile materials (i.e., LEU, HEU, ^{233}U, ^{239}Pu and MOX), based on a subset of criticality experiments chosen from the IHECSBE [3]. Two cross-section libraries were used to establish the overall bias and bias uncertainty for each system, the 238-group ENDF/B-VI and ENDF/B-VII libraries. The results obtained, and summarized in Table 2, also provide a measure of how the cross-section libraries perform, i.e., how accurately the various libraries used in the KENO V.a model can reproduce the experimental results. A combined bias and bias uncertainty value for HEU and LEU systems and for ^{239}Pu and MOX systems has also been reported in Table 2 (last two rows). This combined bias and bias uncertainty was obtained by considering the largest negative bias and largest bias uncertainty from the two combined systems. For example, for the combined HEU and LEU systems, using the 238-group ENDF/B-VI library, the largest negative bias is 0.9946 (from the LEU systems) and the largest bias uncertainty is 0.0056 (from the HEU systems). Hence, the combined bias and bias uncertainty value is 0.9946 ± 0.0056.

By comparing the results of this validation exercise with previous validation work done at AECL for HEU and LEU systems, using the 27-group ENDF/B-IV library, it was concluded that the results using the 238-group ENDF/B-VI or ENDF/B-VII libraries resulted in a smaller k_{eff} bias (i.e., 9 mk for ENDF/B-IV versus 5 mk for ENDF/B-VI and 3 mk for ENDF/B-VII). Furthermore, an improvement was seen in terms of the uncertainties assigned to the bias calculated using the ENDF/B-IV library (i.e., 10 mk), versus the ENDF/B-VI (i.e., 6 mk) and ENDF/B-VII libraries (i.e., 5 mk).

Table 2 Summary of $k_{eff} \pm \sigma$ for SCALE ENDF/B-VI and ENDF/B-VII Libraries

System Type	**238-group ENDF/B-VI**	**238-group ENDF/B-VI**
HEU	0.9965 ± 0.0056	0.9991 ± 0.0046
LEU	0.9946 ± 0.0047	0.9985 ± 0.0038
^{233}U	0.9974 ± 0.0040	1.0000 ± 0.0033
^{239}Pu (fast and thermal energy)	1.0028 ± 0.0042	0.9995 ± 0.0031
^{239}Pu (intermediate energy)	1.0216 ± 0.0200	1.0246 ± 0.0258
MOX	0.9960 ± 0.0028	1.0007 ± 0.0030
^{235}U (combined HEU and LEU)(1)	0.9946 ± 0.0056	0.9985 ± 0.0046
Combined ^{239}Pu and MOX(1, 2)	0.9960 ± 0.0042	0.9995 ± 0.0031

Notes: (1) It is conservative to account for the largest negative bias and the largest uncertainty when combining various systems.
(2) The intermediate-spectrum ^{239}Pu cases are not included in these results.

The results discussed in this paper were also compared with the validation results from ORNL, for the 238-group ENDF/B-V library [4]. The comparison showed that the use of the ENDF/B-VI and ENDF/B-VII libraries resulted in smaller biases and bias uncertainties for all systems. In particular, for HEU systems, the bias uncertainty reported in the ORNL paper for the ENDF/B-V library is 20 mk [4], while that reported in this paper is 6 mk for ENDF/B-VI and 7 mk for ENDF/B-VII. Similarly, for ^{239}Pu systems, the use of the ENDF/B-V library results in a 20 mk [4] bias uncertainty, which is much higher than that reported in this paper (see Table 2).

Important features of the revised validation exercise reported in this paper include:

- The calculated overall k_{eff} value reported in Table 2 accounted for the fact that the nominal benchmark k_{eff} value is different than 1.000;
- The uncertainty for each system included both the experimental and/or modelling uncertainty provided in the benchmark description, as well as the Monte Carlo standard deviation for each modelled critical experiment;
- When available, heavy water experiments were also included in the analysis, to provide useful data applicable to processes at Chalk River Laboratories, which can include the use of heavy water; and
- All systems were modelled based on the benchmark descriptions provided in the IHECSBE [3], and were independently verified.

4. Conclusions

Bias and bias uncertainty results are calculated and reported in this paper for various fissile material systems. The results can be applied to a wide range of systems since the critical experiments chosen cover a wide range of geometries, moderators, reflectors, and energy spectra. Based on the information presented in this paper, the following conclusions can be drawn:

- Acceptability of the SCALE/KENO V.a software for use in criticality safety analysis is confirmed by the close proximity of the computational results to the experimental results reported in the IHECSBE [3].
- The use of the ENDF/B-VI or ENDF/B-VII libraries is recommended for criticality safety analysis, as it results in a smaller bias and bias uncertainty compared to that obtained using other libraries (e.g., ENDF/B-IV or ENDF/B-V).
- The 238-group ENDF/B-VII cross-section library performs better than the ENDF/B-VI library for all types of systems. In particular, the library performs well (i.e., a bias <1 mk) for HEU, ^{233}U, ^{239}Pu and MOX systems. The results are also good for LEU systems, with a slight negative bias of 1.5 mk.
- Both libraries have a poor performance (i.e., positive bias values greater than 20 mk) for the intermediate-energy and mixed spectra ^{239}Pu experiments. In general, there is a scarcity of performed and published critical experiments for mixed and intermediate ^{239}Pu spectra which are not correlated. This lack of un-correlated experiments leads to an under-characterization of the library in the intermediate and/or mixed energy ranges. The code user should exert caution when modelling and analyzing systems in these energy ranges.

5. References

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[4] S.M. Bowman, et. al, “Experience With the SCALE Criticality Safety Cross-Section Libraries”, Oak Ridge National Laboratory, NUREG/CR-6686, ORNL/TM-1999/322 (2000).