Bias between ENDF/B-VIII.0 and ENDF/B-VII.1 for LEU Pin Array Systems*

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INTRODUCTION

Extensive testing of new cross section data is performed in SCALE prior to its release. The release of ENDF/B-VIII.0 [1] requires the generation and testing of new data libraries which are planned to be included in the release of SCALE 6.3 in 2019 or 2020. KENO [2] benchmark results have been published previously for beta and final releases of ENDF/B-VIII.0 [3,4] using the entire Verified, Archived Library of Inputs and Data (VALID) [5]. This work presents an energy-dependent change in the results for low-enriched uranium (LEU) pin array systems. The process of identifying the difference is highlighted as a case study to determine how data testing and benchmarking can be performed to provide more detailed feedback to the data community on potential data deficiencies.

VALID LIBRARY

The VALID library contains over 600 individual benchmark experiment configurations drawn from 14 different categories in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [6]. The majority of these cases use KENO V.a, but 57 cases use KENO-VI. The 14 categories represented in the library include high-enriched uranium fast metal (HMF) systems, high-enriched uranium thermal solution (HST) systems, intermediate-enriched uranium fast metal systems (IMF), LEU thermal compound systems (LCT) systems, LEU thermal solution (LST) systems, mixed U/Pu fast compound (MCF) systems, mixed U/Pu thermal compound (MCT) systems, mixed U/Pu thermal solution (MST) systems, plutonium fast metal (PMF) systems, plutonium thermal solution (PST) systems, ^{233}U thermal compound (UCT) systems, ^{233}U fast metal (UMF) systems, ^{233}U intermediate spectrum solution (USI) systems, and ^{233}U thermal solution (UST) systems. KENO-VI cases come from only three categories: HMF, IMF, and MCT. The evaluations used are described in the complete validation report [7]. A total of 140 LCT cases are included in VALID and are drawn from the LCT-001, -002, -008, -010, -017, -042, -050, -078, and -080 evaluations.

LCT RESULTS SUMMARY

The results presented here were generated with SCALE 6.3 beta 3, a primarily internal preliminary beta release at Oak Ridge National Laboratory (ORNL). The code release was intended to allow early testing by internal users at ORNL. The full suite of VALID results using continuous-energy libraries based on ENDF/B-VII.1 [8] and ENDF/B-VIII.0 [1] is summarized in Marshall et al. [4]. The average calculation-to-evaluation (C/E) ratio for the ENDF/B-VII.1 library is 0.99959 ± 0.00018, and for the ENDF/B-VIII.0 library, it is 0.99915 ± 0.00018, resulting in a slightly larger magnitude bias for the ENDF/B-VIII.0 library. The increase from 0.00041 Δk to 0.00085 Δk only represents approximately 1.7 standard deviations, so it may not even be considered statistically significant. All 140 C/E ratios for both the ENDF/B-VII.1 and ENDF/B-VIII.0 libraries are shown in Figure 1. Figure 1 includes dotted lines showing the uncertainty in the C/E ratio, accounting for experimental and stochastic uncertainties, and dashed lines for the nuclear data-induced uncertainty in k_{eff} based on multigroup TSUNAMI-3D calculations. A detailed review of the differences between the data sets starts with a careful examination of this data.

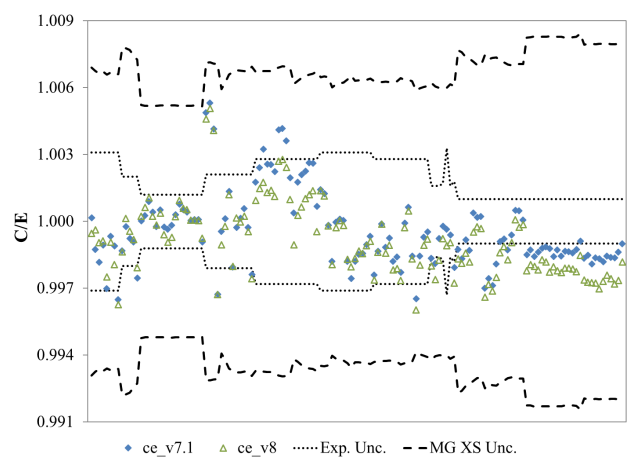

Figure 1. C/E ratios for all 140 LCT systems.

DETAILED REVIEW OF RESULTS

The differences between the ENDF/B-VII.1 and ENDF/B-VIII.0 results shown in Figure 1 are generally small, which is expected given the small magnitude of the change in the average C/E ratio. Also as expected, the C/E ratios for the ENDF/B-VIII.0 library tend to be slightly lower than those for the ENF/B-VII.1 results. There are two areas where the ENDF/B-VIII.0 C/E ratios are noticeably lower than the ENDF/B-VII.1 results, as indicated by the red boxes in Figure 2. The region near the

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middle of the plot corresponds to LCT-010 cases 14–30, and the region at the right side of the figure corresponds to LCT-078 and -080. A review of the LCT-010 evaluation [6] shows that cases 1–13 have a 2.54 cm pitch, while cases 14–30 have a 1.892 cm pitch. LCT-078 and -080 are also both relatively tight-pitch experiments, though the fuel rods are also much smaller than those used in LCT-010.

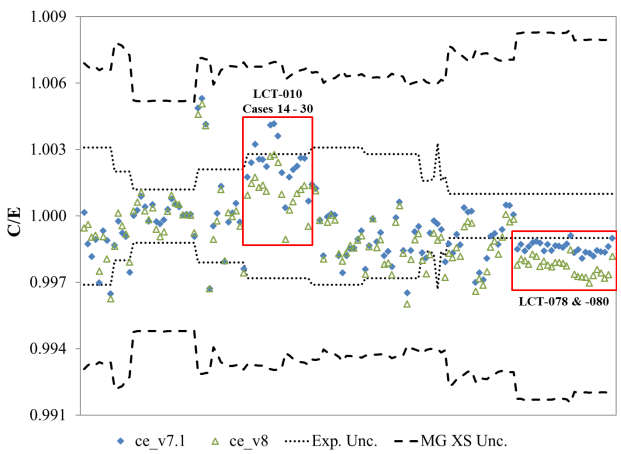

Figure 2. C/E ratios with differences highlighted.

The reduced pitch present in the cases with larger differences may indicate a bias as a function of moderation/neutron energy spectrum. KENO reports the energy of the average lethargy causing fission (EALF) with each calculation, so this spectral measure is typically used at ORNL based on convenience. The SCALE 6.2.2 validation report [7] presented C/E ratios as a function of EALF for each system category; no trend was noted for the libraries considered in that report. Figure 3 shows the calculated k_{eff} values for both ENDF/B-VII.1 and ENDF/B-VIII.0 libraries as a function of EALF. The raw k_{eff} values are used instead of the C/E ratios because the evaluated k_{eff} is the same for both models. The differences in C/E ratios are therefore equivalent to the differences in the k_{eff} values.

As with the SCALE 6.2.2 validation report, no clear trend is evident in the results for either library. It is interesting to note, however, that there are larger differences between the ENDF/B-VII.1 and ENDF/B-VIII.0 results at higher EALF values than at lower EALF values. This is particularly evident for the series of 6 points at EALFs from 0.43 to 0.61 eV and k_{eff} values near or above 1.0. These points come from LCT-010 and are cases 25–30, which are 6 of the 7 uranium-reflected cases with the 1.892 cm pitch. Case 24 is the other case, and it has the reflecting wall positioned farther from the fuel arrays. The larger separation distance allows more water to be close to the arrays, reducing the EALF value to approximately 0.38 eV. Another group of noticeable points is at an EALF of approximately 0.475 eV, with C/E ratios between 0.994 and 0.998. The differences between ENDF/B-VII.1 and ENDF/B-VIII.0 are larger for these points than for most of the points at lower EALFs. These points are from LCT-080, cases 1–10. Case 11 has empty lattice locations to simulate fuel assemblies, so it has a significantly softer spectrum. These observations indicate that there may be an energy-dependent bias in the *differences* between the two libraries, even if there is no clear energy-dependent bias in either library.

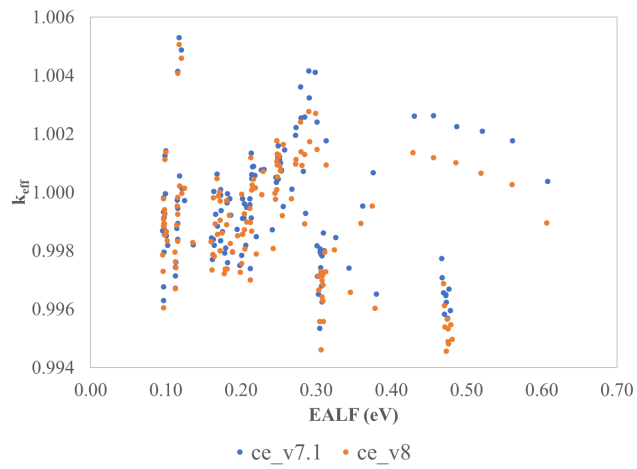

Figure 3. C/E ratios as a function of EALF.

The difference in the calculated k_{eff} values between ENDF/B-VIII.0 and ENDF/B-VII.1 is shown in Figure 4. There is a clear trend in the differences between the results from the two libraries. As the spectrum gets harder, the ENDF/B-VIII.0 library yields more negative results. The average C/E ratio is lower for ENDF/B-VIII.0, as discussed previously, but now it is evident that this is driven by a bias that becomes more pronounced with slightly harder neutron energy spectra.

Further investigation shows that the trend is consistent within several LCT evaluations and is not just an artifact of differences between evaluations. Figure 5 presents the same data as Figure 4, but each evaluation is shown separately. LCT-010, -017, -078, and -080 all cover a broad enough range in EALF to exhibit a negative bias between cases within the evaluation. Both LCT-078 and -080 have a final case with water-filled lattice locations to simulate the guide tubes in a pressurized-water reactor fuel assembly. The introduction of these water holes dramatically softens the system spectrum. LCT-008 is the only evaluation that does not show a negative bias with what might be considered a broad enough variation in neutron energy spectra; the 17 cases in LCT-008 do not manifest any clear trend as a function of EALF. The overlap between the LCT-010 and -017 results provides additional confirmation of the trend.

Further investigation of the results of these LCT systems and other systems is needed to understand the

likely causes for this bias. The HST and LST systems in VALID may provide further insight, but the LST systems have a very small variation in neutron energy spectra. The HST systems may be more useful, especially in trying to determine if the bias is likely a result of changes to ^{235}U or ^{238}U.

CONCLUSIONS

A detailed comparison of C/E ratios for LCT systems in the VALID library was presented. This detailed examination led to the discovery of an energy-dependent bias between the ENDF/B-VIII.0 and ENDF/B-VII.1 results. The overall lower bias for ENDF/B-VII.1 indicates that the ENDF/B-VIII.0 bias indicates poorer performance and should be fixed if possible. This paper also presents the process whereby the bias was discovered. No in-depth knowledge of the benchmark experiments present in the VALID library was necessary to identify this bias, though such knowledge can accelerate the investigation. Ultimately, more systems must be examined, possibly with a broader set of tools, to determine the likely cause of the bias presented here.

ACKNOWLDGMENT

The US Department of Energy Nuclear Criticality Safety Program (NCSP) sponsored this work and the preparation and presentation of this paper.

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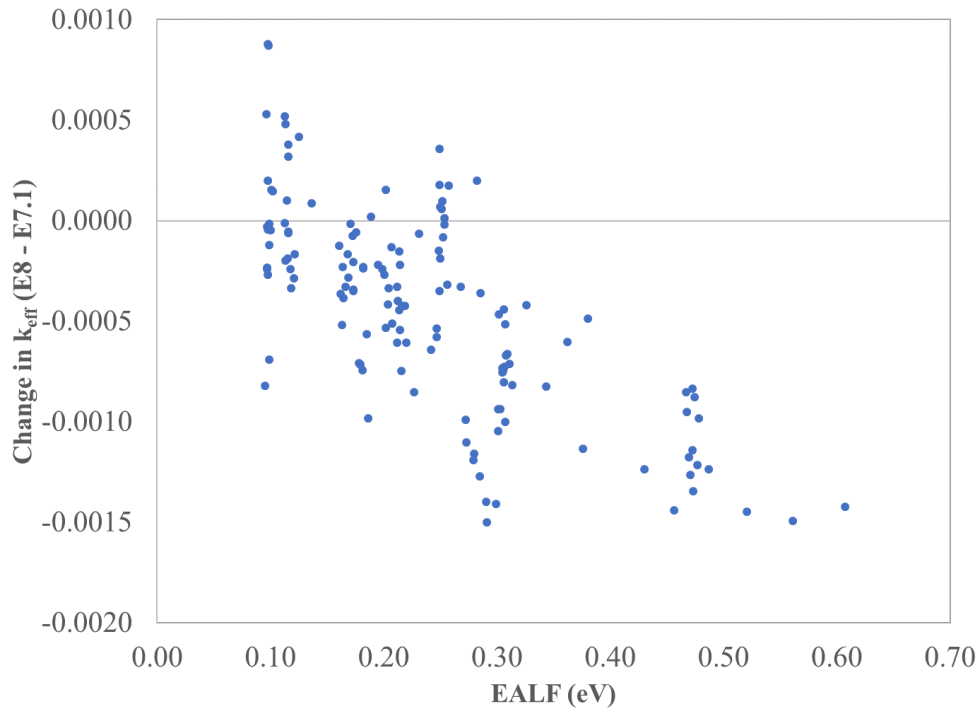

Figure 4. Change in k_{eff} as a function of EALF.

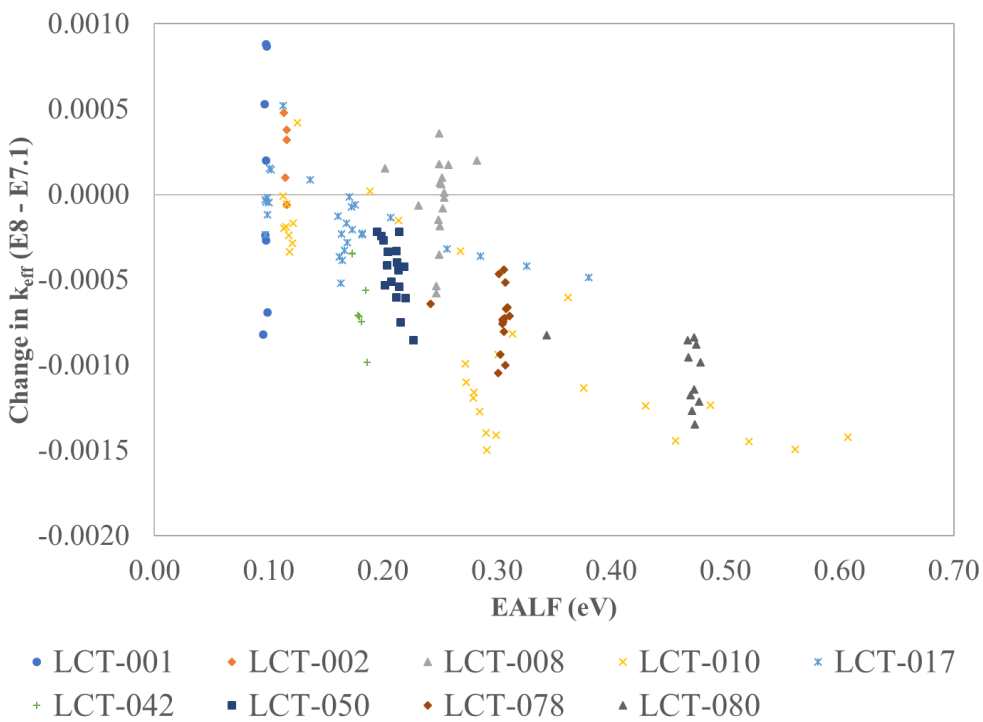

Figure 5. Change in k_{eff} as a function of EALF, by evaluation.