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ENDF/B-VII Nuclear Data Libraries for SCALE 6

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INTRODUCTION

Version 6 of the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system [1] was released in February 2009. SCALE provides a comprehensive, integrated package of modular programs and nuclear data for a wide range of applications, including reactor physics, criticality safety, shielding, sensitivity/uncertainty analysis, and isotopic transmutation and radiation source term determination. SCALE computational modules are executed by automated *control sequences* that prepare input and call the desired modules in a particular order, linking output from one calculation to the next in series. The SCALE lattice physics sequence TRITON generates few-group, assembly-homogenized cross sections, as a function of burnup and branch states, which can be input to core simulator codes. TRITON couples the ORIGEN-S depletion module with either the NEWT (NEW Transport algorithm) two-dimensional (2D) arbitrary-geometry transport code or the three-dimensional Monte Carlo KENO code. Fluxes from the transport solution, along with self-shielded multigroup (MG) cross sections, are passed to ORIGEN-S, which computes the time-dependent isotopic concentrations of more than 1400 nuclides.

One of the major advancements in SCALE 6 is the availability of new nuclear data libraries based on ENDF/B-VII [2] for neutron transport calculations. In this paper we describe the SCALE ENDF/B-VII (designated here as V7) libraries and present some validation results for critical benchmarks and isotopic depletion experiments.

ENDF/B-VII NUCLEAR DATA LIBRARIES

SCALE 6 includes both pointwise (PW) and MG libraries processed from the ENDF/B-VII nuclear data files by the AMPX code system [3]. The PW data are used for two distinct functions. First, they are used for continuous-energy (CE) Monte Carlo calculations with KENO. Second, they are used in the one-dimensional CENTRM CE discrete ordinates code to compute spectral fine structure for self-shielding MG cross sections. The PW nuclear data are stored on a very fine energy mesh so that the value at any energy can be linearly interpolated with an error less than 0.1%. For example, the PW capture cross section of ^{238}U at room temperature contains about 150,000 energy points. SCALE 6 includes PW data files for all reactions of all materials available in the ENDF/B-VII evaluated nuclear data files (~390 materials) at several different temperatures.

The V7 MG library in SCALE has 238 energy groups. MG cross sections and transfer arrays were processed by AMPX from the PW data of each material using a generic weighting function. During lattice physics calculations, the 238 fine-group library is typically collapsed using problem-specific fluxes to a coarser group structure (default is 49 groups) for use in the TRITON 2D lattice physics calculations with burnup. MG cross sections in the thermal and resolved resonance ranges are recomputed by the PMC code, which combines the PW fluxes computed by CENTRM and the PW V7 nuclear data to obtain problem-specific, self-shielded cross sections for MG transport and depletion calculations.

VALIDATION STUDIES FOR CRITICAL BENCHMARKS

The SCALE 6 V7 libraries were validated by analyzing approximately 1300 criticals using CE and MG Monte Carlo computations with KENO. Reference [4] describes results obtained with CE KENO. In this paper MG results are presented for low-enriched uranium (LEU) and mixed oxide (MOX) benchmarks and are compared with experimental and CE Monte Carlo values.

Fig. 1 shows ratios of calculated-to-experimental (C/E) values of k_{eff} obtained for 318 LEU benchmarks in this set. In general, the agreement between the V7 calculations and experiments is good and has been improved over earlier results obtained with ENDF/B-VI.8. Overall the MG values show a bias of about 1–2 milli-k as compared to the CE results. In most cases, calculated values lie within the combined Monte Carlo and experimental uncertainty (typically ± 3 mill-k); however, the calculated values for two series of benchmarks are noticeably low. As shown in Fig. 1, MCNP results from reference [5] are similar to those from SCALE for these cases. The discrepancy is most likely due to uncertainties in the experimental specifications given in the International Criticality Safety Benchmark Evaluation Program (ICSBEP) Handbook. [6]

Fig. 2 shows the k_{eff} C/E ratios obtained using MG- and CE-KENO for 83 thermal and fast MOX criticals. MCNP results from reference [2] are also shown for selected cases. The ICSBEP benchmark models for several of these critical facilities have reactivity uncertainties in the range of 500–700 pcm.

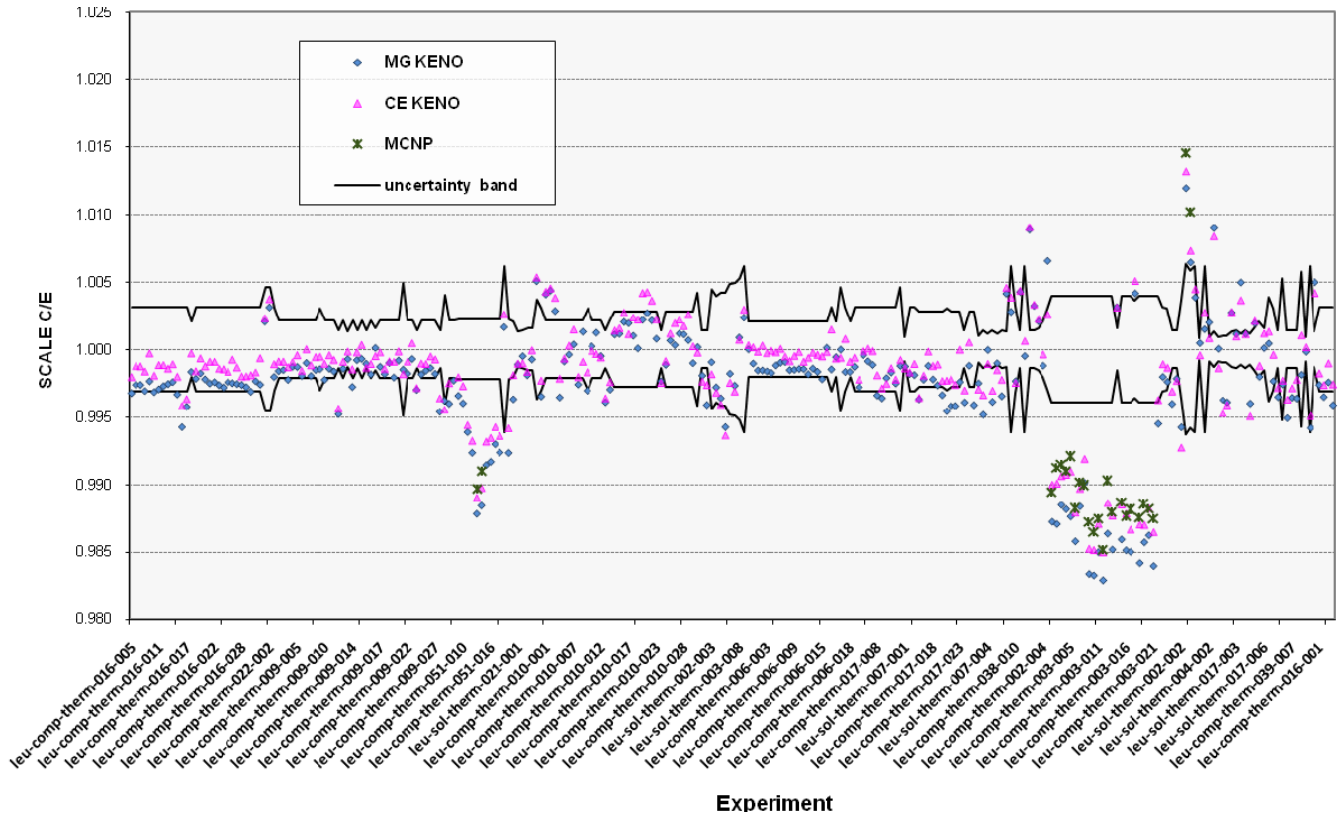

Fig. 1. C/E values of k_{eff} for LEU benchmark criticals.

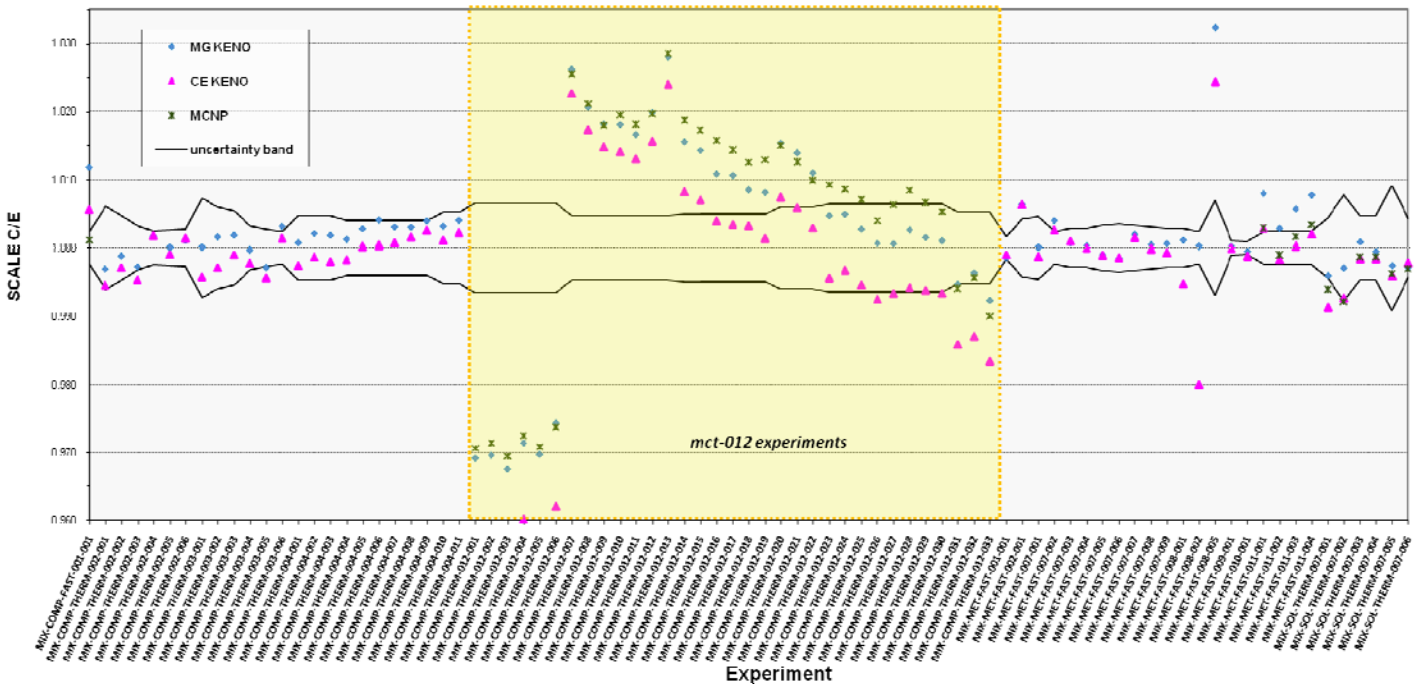

Fig. 2. C/E values of k_{eff} for MOX benchmark criticals.

Except for the MOX thermal experiment series designated as MCT-012 in the ICSBEP handbook, the computed values are generally within the experimental uncertainties. Although there is some variation among the three methods, the calculated eigenvalues for many of the MCT-012 cases show large discrepancies as compared to the experimental results. The poor agreement obtained using ENDF/B-VII is similar to that for ENDF/B-VI. It is quite possible the discrepancies are due to errors in experimental specifications such as Pu isotopics. New integral measurements for a modern MOX critical with smaller experimental uncertainties are desirable.

VALIDATION STUDIES FOR PWR ISOTOPIC MEASUREMENTS

The new libraries were also validated by comparing TRITON/NEWT calculations for the isotopic content in spent nuclear fuel with experimental radiochemical assay data. A database of isotopic measurement data has been compiled and documented at Oak Ridge National Laboratory as part of a sustained validation effort to determine the isotopic bias and uncertainty in spent fuel calculations for the actinides and fission products of importance to spent fuel safety applications. This database includes radiochemical assay data acquired from domestic and international experimental programs and covers a large range of burnup and fuel enrichment values. The most recent radiochemical isotopic assay data set was acquired through the MALIBU international program.[6] This program was designed to provide a large set of reliable, high-quality experimental isotopic data with low uncertainties for high burnup commercial spent nuclear fuel; the spent fuel measurements for the first phase of the program, which were carried out between 2004 and 2006 at three different laboratories, included extensive actinide and fission product data. Cross-check measurements were performed for some of the analyzed spent fuel samples to reduce the experimental uncertainties and improve confidence in the measured data. The measurement data obtained in the MALIBU program for three uranium oxide (UO_2) spent fuel samples are used in the current paper to assess the performance for depletion analysis of the new ENDF/B-VII library available in SCALE 6. The UO_2 samples were selected from the same fuel rod, with 4.3 wt% ^{235}U initial enrichment, which was irradiated in a pressurized water reactor. The samples had burnups of approximately 70, 51, and 46 GWd/MTU, respectively. These measurements were previously analyzed with SCALE 5.1 using libraries based on ENDF/B-V data. [7]

The computational analysis of the measurements was carried out using the SCALE depletion sequence TRITON/NEWT that couples the NEWT transport code with the isotopic depletion and decay code ORIGEN-S to perform the burnup simulation. At each depletion step, the transport flux solution from NEWT is used to generate cross sections for the ORIGEN-S calculation; the isotopic composition data resulting from ORIGEN-S are employed in the subsequent NEWT transport calculation to obtain cross sections for the next depletion step in an iterative manner throughout the irradiation history. The TRITON model used for the current study is similar to the model previously used [7] for analysis of these measurements with SCALE 5.1. However, whereas the previous analysis employed the SCALE 44-group ENDF/B-V cross-section library (designated here as V5) and the NITAWL self-shielding module, the analysis presented in the current paper used the new SCALE 238-group cross-section library based on V7 data and the CENTRM/PMC self-shielding methodology. Cross-section data for 232 isotopes available in the multigroup transport library were self-shielded and then collapsed using the spectrum calculated by NEWT at each burnup step. These updated cross sections were passed to the ORIGEN-S fuel depletion calculation. Nuclear data for the remaining isotopes in the depletion calculation were taken from the standard ORIGEN-S three-group library.

The comparison of the calculated and measured isotopic concentrations for the three samples considered is illustrated in Figs. 3–6 for both SCALE libraries used (i.e., SCALE 6 V7 and SCALE 5.1 V5). For each nuclide, the plotted data show the values of (C/E-1) in percentage, where C/E represents the C/E concentration ratio. As seen in Fig. 3, the overall agreement of calculation and measurement for uranium and plutonium isotopes is similar for both SCALE libraries. When V7 is used, ^{235}U and ^{239}Pu are on average calculated within 0.4 and 1.3% , respectively, of the measured data. In the case of minor actinides (Fig. 4), V7 yields a large improvement of about 30% on average in the results for ^{245}Cm and ^{246}Cm, isotopes important for neutron source term calculations.

Results for the samarium isotopes (Fig. 5) are much better with V7 than with V5, notably ^{147}Sm, ^{149}Sm, ^{151}Sm, and ^{152}Sm, which are fission products with large absorption cross sections. The ^{149}Sm isotope, one of the most important fission products for reactor analysis and burnup credit, is calculated on average within 4% of the measured data with V7, as compared to within 12% with V5. Large improvements of approximately 20% for V7 compared to V5 results are also seen in the estimations of ^{151}Sm and ^{152}Sm .

The calculation-versus-measurement agreements for europium and gadolinium isotopes are significantly improved using V7 (Fig. 6). For example, in the case of ^{153}Eu and ^{155}Gd, both fission products important to burnup credit, the average C/E improves from 5.6 and –29% with V5 to 0.4 and –1% with V7, respectively. Another significant improvement in estimation of fission products with V7 (not shown in a plot here) was observed in the case of ^{134}Cs, an important gamma emitter and major

contributor to decay heat for short cooling time. In this case, the average C/E changed by about 10%, from –14% with V5 to –4% for V7.

SUMMARY

Version 6 of the SCALE code system includes new ENDF/B-VII PW and MG nuclear data libraries for a variety of applications, including reactor lattice physics calculations, source term analysis, and spent fuel characterization. The codes and nuclear data libraries have been validated against critical experiments and isotopic measurements. Overall, LEU critical experiments are computed better with V7 than with earlier versions of ENDF/B. The k_{eff} values calculated with V7 for MOX criticals generally agree within the experimental error of measured results, except for the MCT-012 series which shows a wide variation compared to the values given in the ICSBEP. Much of the discrepancy is likely caused by uncertainties in the experiment specifications. Numerous HEU and Pu critical benchmarks were also analyzed and show similar good results.

For the spent fuel isotopic measurements studied here, the major actinide concentrations are computed with the ENDF/B-VII libraries to an accuracy similar to that obtained with earlier SCALE computations using ENDF/B-V, which is acceptable agreement considering the experimental uncertainty. Curium isotopic results are greatly improved with ENDF/B-VII. Several important samarium, europium, and gadolinium fission product isotopes are also calculated significantly better with V7.

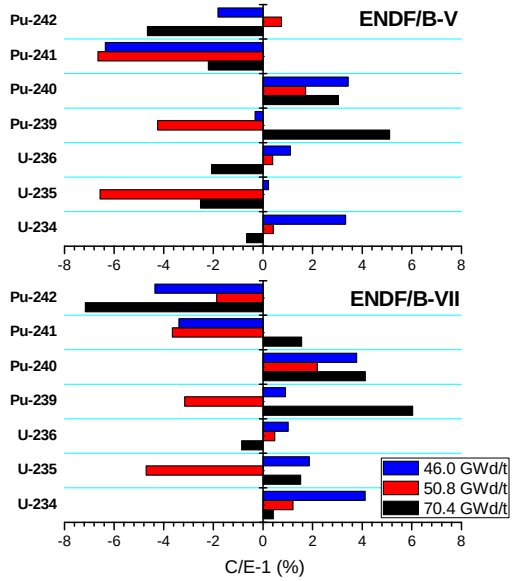

Fig. 3. Calculated-experimental results for major actinides.

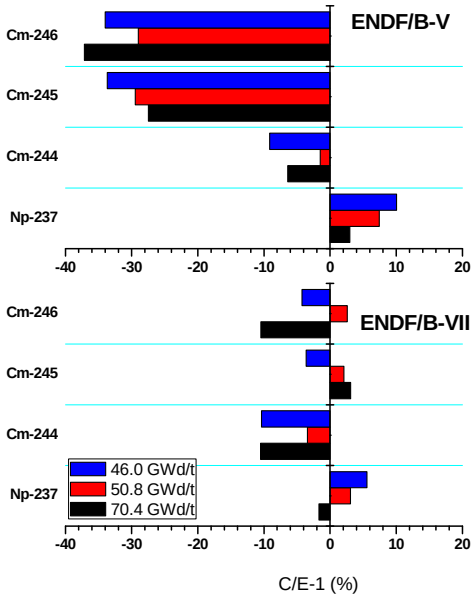

Fig. 4. Calculated-experimental results for minor actinides.

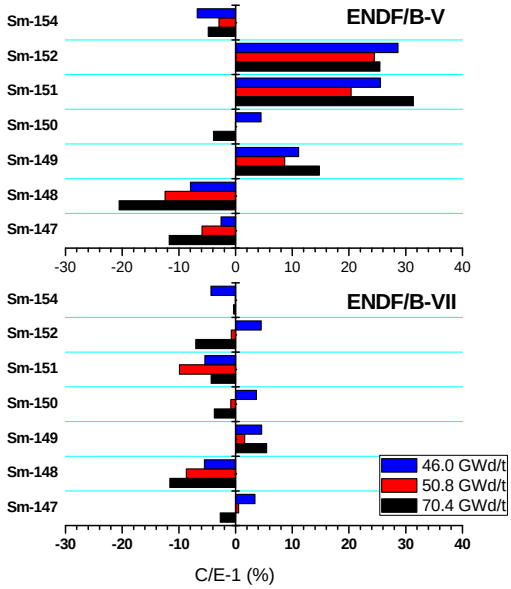

Fig. 5. Calculated-experimental results for Sm isotopes.

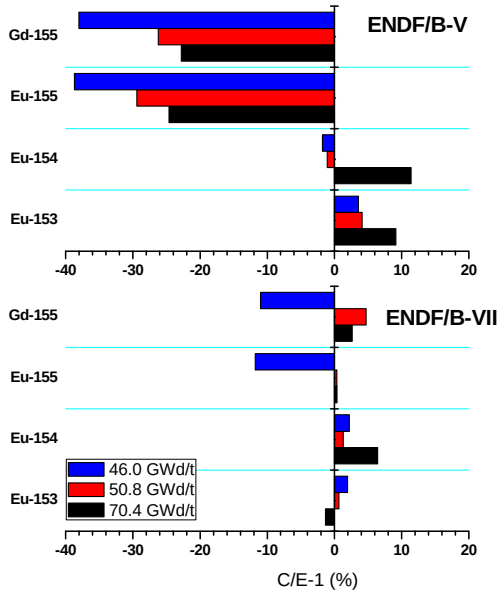

Fig. 6. Calculated-experimental results for Eu and Gd isotopes.

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