Testing New Actinide Cross Sections Proposed for ENDF/B-VII

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Abstract. Our Nuclear Physics Group has worked over the last several years to improve the ENDF/B actinide cross sections, especially as measured against the famous series of fast-spectrum critical experiments performed at Los Alamos under such names as Godiva, Jezebel, the Flattops, and Bigten. The new evaluations include changes in the high-energy fission cross sections, nubar, elastic scattering, inelastic scattering, fission spectra, and delayed neutrons that combine to significantly improve the calculated results for the Los Alamos critical assemblies. As a happy byproduct of this work, we found that the new evaluations also removed about half of a long-standing discrepancy in calculations of thermal-reactor critical experiments using lattices of low-enriched uranium oxide rods. In the meantime, work at the Oak Ridge National Laboratory has resulted in new proposed resonance parameters for U238. When these low-energy data are combined with the new high-energy data from Los Alamos, they have the effect of removing most of the rest of the problem for thermal lattices. Although more work will be done at both Los Alamos and Oak Ridge, including making the evaluations consistent with the new standards, the results presented in this talk provide promise that ENDF/B-VII will result in good improvements for users at both high and low neutron energies.

INTRODUCTION

One measure of the quality of a set of nuclear data evaluations, such as the current version of the US standard Evaluated Nuclear Data Files (ENDF/B-VI Release 8), is to use it to calculate models of critical experiments. In order to draw good conclusions about the data, it is important that the critical assemblies be clean, simple, and well characterized. In the fast energy region (say 1 keV to 12 MeV), the famous series of Los Alamos criticals, including Godiva, Jezebel, the Flattops, and Bigten, fill this role nicely. It is natural that our Nuclear Physics Group would work to improve the evaluations of actinide isotopes in order to improve the predictions for these critical assemblies. This work was done in an iterative manner using the results of calculations to help guide the choice of evaluation options, to focus on important classes of data, and to help choose between disparate data. We would then repeat the calculations to check that the new evaluations had the desired effects and continue the iteration. The end result is a new set of actinide evaluations being proposed for ENDF/B-VII with improved high-energy cross sections that fairly well satisfies our goal[1]. When we attained this milestone, we combined our new high-energy evaluations with new resonance-range evaluations from ORNL[2] and extended our testing to thermal critical assemblies with good results.

THE PRE-VII EVALUATIONS

The new actinide evaluations include the isotopes of uranium from 232 through 241, Pu239, and Np237, but not all of these materials are included in the critical assemblies tested here. The evaluations include changes in the high-energy fission cross sections, nubar, elastic scattering, inelastic scattering, fission spectra, and delayed neutrons. For U235, the most important change for the purposes of this report was an increased fission cross section in the 1.5 to 4 MeV range. This change echoed to all the other materials through the well measured fission ratios. Some corresponding changes to nubar were also made at this time, and they affected the criticality results also. For U238, changes in the elastic scattering cross sections and angular distributions were important for the reflectors in the Flattop and Bigten assemblies. The new calculations for inelastic scattering in U233 and U238 were very significant in correcting very large discrepancies in Jezebel-23 (a bare U233 sphere) and Bigten (with approximately 10% enrichment in its core). The basic Los Alamos evaluations with their improved high-energy representations were made available for testing at *http://t2.lanl.gov/data/data/preVII-neutron* in subdirectories *U, Np, Pu* with names like 238l. Later versions with new resonance-range treatments from ORNL were included in the web area with the suffix "o", *e.g.*, 238o.

FAST CRITICALS

Table 1 compares experiment and calculations made with MCNP5[3] using both the new preVII cross sections as processed by the NJOY Nuclear Data Processing System[4] and the previous cross sections based on Release 8 (which are .66c materials with .62c for oxygen in the cross section libraries distributed with MCNP5). The statistical accuracy of the Monte Carlo cross sections is about .0002 (one sigma). When possible, two different models were used for each assembly. The cases with spelled out names (such as “Godiva” or “Bigten”) are from the Cross Section Evaluation Working Group (CSEWG) Benchmark Handbook[5]. CSEWG manages the ENDF system. The case “HMF001” (HEU-Metal-Fast) is the version of Godiva from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSB)[6], and other similarly named cases are also from this important compilation. To summarize, Godiva (and HMF001) is a bare sphere of U235, Jezebel (and PMF001) is a bare sphere of Pu239, Flattop-25 (HMF028) is a sphere of U235 reflected by natural uranium, Flattop-Pu (PMF006) is a sphere of Pu239 reflected by natural uranium, Jezebel-23 (UMF001) is a bare sphere of U233, Flattop-23 (UMF006) is a sphere of U233 reflected by natural uranium, Bigten has a composite core of interleaved plates of enriched and natural uranium with an effective enrichment of about 10% reflected by natural uranium, and the “Bigten” model used here is homogenized and spherical. The two IMF cases are additional more complex models for Bigten, one a two-dimensional model with homogenized regions, and the other a detailed plate model of the assembly. PMF011 is a sphere of Pu239 reflected by water, and HMF004 is a sphere of U235 reflected by water.

Godiva and Jezebel results show good k-eff values as a result of the changes in fission and nubar. For many years, the k-eff values for reflected assemblies have computed quite a bit higher than for the corresponding bare assemblies. This “reflector bias” has been reduced quite a bit, largely due to the changes in U238 elastic scattering in the MeV range. The improvement in Jezebel-23 and Flattop-23 is dramatic, mostly resulting from the sophisticated new inelastic analysis. The improvement in Bigten is also dramatic, mostly resulting from the new inelastic data in the U238 evaluation. The simple spherical CSEWG model and the more complex ICSB models seem to agree fairly well.

Another valuable feature of the Los Alamos fast critical assemblies is that additional experimental measurements beyond k-eff are available. One especially useful set of measurements is the fission ratios or “spectral indices” made by inserting small fission chambers into the assemblies. The ratio of the U238 fission rate to the U235 fission rate tends to tell you what fraction of the flux is above the 1 MeV fission threshold for U238. Some results are shown in Table 2.

TABLE 1. MCNP5 Calculations for k-eff of Some Fast Critical Assemblies Compared to Experiment

Assembly Name	Release 8 k-eff C/E	preVII k-eff C/E
Godiva	.9967	.9997
HMF001	.9966	.9994
Jezebel	.9972	1.0005
PMF001	.9975	1.0002
Flattop-25	1.0019	1.0030
HMF028	1.0015	1.0033
Flattop-Pu	1.0028	1.0019
PMF006	1.0020	1.0013
Jezebel-23	.9926	.9988
UMF001	.9926	.9986
Flattop-23	1.0024	1.0006
UMF006	1.0006	.9986
Bigten	1.0136	1.0011
IMF007h	1.0125	.9999
IMF007s	1.0117	.9991
PMF011	.9972	.9991
HMF004	.9963	1.0000

TABLE 2. U238/U235 Fission Ratio in LANL Assemblies as Calculation/Experiment

Assembly Name	Release 8 238f/235f C/E	preVII 238f/235f C/E
Godiva	.965	.965
Jezebel	.968	.977
Jezebel-23	1.011	.985
Flattop-25	.981	.971
Flattop-Pu	.986	.982
Flattop-23	.999	.980
Bigten	1.041	.968

The low value for Godiva of .965 suggests that the U235 inelastic scattering treatment might be producing a spectrum that is slightly too soft. The very good values for Jezebel-23 and Flattop-23 were obtained with more advanced theoretical methods than those used for the current U235 evaluation, which suggests that a future new evaluation for U235 might do better on these spectral indices. For Bigten, the U238/U235 fission ratio goes from being 4% too large to being 3% too small, but the small result is more like the small result in Godiva and Flattop-25, thus making the set of results more self consistent.

In addition to the central reaction rate ratios, there also exist less often utilized reaction rate ratios measured at various radii in some of the Los Alamos critical assemblies using radiochemical techniques. The neutron spectrum gets softer as one moves out from the center of the assembly, thereby giving additional information

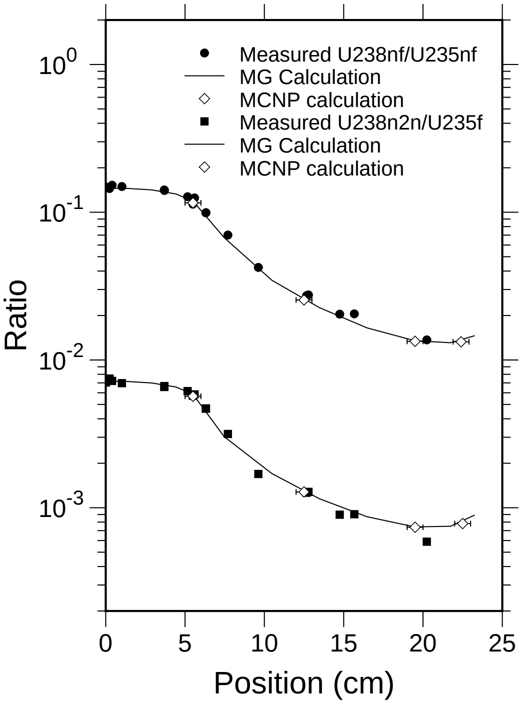

FIGURE 1. Comparison of experimental radiochemical data from Flattop-25 and Topsy with calculated values for a radial traverse in the Flattop-25 assembly. The ratio of the U238(n,f) reaction rate to the U235(n,f) reaction rate and the ratio of the U238(n,2n) reaction rate to the U235(n,f) reaction rate are plotted versus radius.

about the quality of the cross section data. An example of these data as taken in the Flattop-25 and Topsy assemblies is shown in Figure 1. (Topsy was an early mockup of a U235 core reflected by natural uranium made by stacking cubes of material—its geometry is not as clean as the later Flattop experiment.) The calculations were done using multigroup methods based on MATXS cross sections from NJOY[4] formatted with TRANSX[7] for PARTISN[8]. A very fine group structure with 1/16-lethargy intervals in the fast region was used for high accuracy. The multigroup results were checked by tallying in several 1-cm shells using MCNP5, and good agreement was obtained. Figure 2 shows a different presentation of these data in a form often used by radiochemists. The abscissa is a measure of the hardness of the spectrum, and this kind of plot often allows data from different assemblies to be compared on a common basis. This is demonstrated here using data from Flattop-25 and Topsy. Note how the calculated central ratio for Bigten also fits into this kind of plot.

These calculated results show a slight hardening of the neutron spectrum at the outer edge of the reflector (24cm for Flattop, 26cm for Topsy)) that doesn’t seem to be supported by the measurements. This might suggest additional possible improvements that could be made in a future new evaluation for U238.

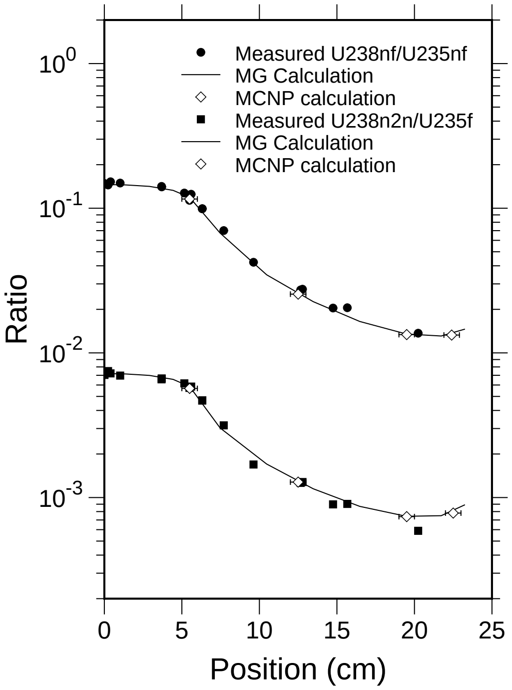

FIGURE 2. Comparison of experimental radiochemical and calculated values for radial traverses in the Flattop-25 and Topsy assemblies. The ratio of the U238(n,2n) reaction rate to the U235 fission rate is plotted against the ratio of the U238 fission rate to the U235 fission rate for different positions (with central positions to the right and positions in the reflector to the left). The abscissa is a measure of the hardness of the spectrum at that position. The Bigten result is computed at the center of the assembly.

THERMAL SOLUTION CRITICALS

With Release 8 of ENDF/B-VI, it was felt that calculations of solutions of highly-enriched uranium were being handled very well. The k-eff values were good, and the biases in k-eff with parameters such as leakage or above-thermal-fission fraction that plagued earlier versions were gone. When the new preVII evaluations became available, we carried out a number of calculations to verify this feeling and to make sure that the new data don’t damage the good level of agreement already obtained. MCNP5 results are shown in Tables 3, 4, and

TABLE 3. Low-Leakage Nitrate Solutions

Assembly Name	Leakage	Release 8 k-eff C/E	preVII k-eff C/E
HST042-1	.125	1.0013	1.0017
HST042-2	.128	.9999	1.0002
HST042-3	.071	1.0010	1.0009
HST042-5	.033	.9992	.9993
HST042-7	.026	1.0004	1.0006
HST042-8	.013	1.0012	1.0010
Average		1.0005	1.0006

TABLE 4. Mid-Leakage Nitrate Solutions

Assembly Name	Leakage	Release 8 k-eff C/E	preVII k-eff C/E
HST001-1	.450	.9996	.9996
HST001-2	.460	.9962	.9970
HST001-3	.448	1.0028	1.0031
HST001-4	.458	.9979	.9988
HST001-5	.384	1.0000	1.0002
HST001-6	.391	1.0032	1.0035
HST001-7	.449	.9983	.9997
HST001-8	.450	.9985	.9997
Average		.9996	1.0000

5 with one-sigma statistical accuracies of about .0001, .0003, and .0002, respectively. It is clear that both the old and new cross sections perform very well, and the absence of any bias with leakage is demonstrated.

We then extended our testing to include some low-enriched uranium solution criticals in order to test whether the higher concentration of U238 would reveal any new problems. The results in Tables 6 and 7 show that both sets of cross sections perform very well for these assemblies, and there is no evidence of any bias with respect to leakage. The one-sigma statistical error for these case is about .0002.

TABLE 5. High-Leakage Fluoride Solutions

Assembly Name	Leakage	Release 8 k-eff C/E	preVII k-eff C/E
HST009-2	.469	1.0006	1.0005
HST009-3	.472	1.0001	1.0005
Average		1.0003	1.0005

TABLE 6. Unreflected Low-Enriched Uranium Solution Experiments

Assembly Name	Leakage	Release 8 k-eff C/E	preVII k-eff C/E
LST007-1	.223	.9984	.9992
LST007-2	.208	1.000	1.0004
LST007-3	.192	.9971	.9980
LST007-4	.176	.9992	1.0004
LST021-1	.177	.9992	1.0000
LST021-2	.158	.9996	.9999
LST021-3	.132	.9983	.9989
LST021-4	.114	.9996	1.0000
Average		.9989	.9996

TABLE 7. Reflected Low-Enriched Uranium Solution Experiments

Assembly Name	Leakage	Release 8 k-eff C/E	preVII k-eff C/E
LST004-1	.221	1.0001	1.0009
LST004-2	.205	1.0008	1.0018
LST004-3	.190	.9991	1.0002
LST020-1	.177	1.0000	1.0005
LST020-2	.158	.9997	1.0000
LST020-3	.131	.9987	.9990
LST020-4	.063	.9997	1.0004
Average		.9997	1.0004

THERMAL LATTICES

For many years, calculations for critical lattices of low-enriched uranium oxide rods in water have shown a substantial under prediction of k-eff. This is important, because these assemblies are prototypical of real nuclear power reactors. Manufacturers and operators of nuclear power systems have had to resort to making adjustments in their proprietary data libraries to compensate for this shortcoming in the evaluated nuclear data libraries. When we tested our new high-energy evaluation for U238 against some thermal lattices, we saw a significant improvement in the results that we credited to the new inelastic scattering treatment. Later, when a new preliminary evaluation of the U238 resonance parameters became available from Oak Ridge, we found that the combination of the two effects came pretty close to removing the classical underprediction of k-eff. Table 8 gives results for a series of lattice experiments done in Japan with variations in the arrangement of the rods. The preVII data give k-eff values within experimental error and, as shown by the reduction in the scatter, also reduce the biases coming from different arrangements. The one-sigma statistical error for these calculations is about .00025.

In Tables 9 and 10, calculations are shown for some uranium-oxide rod lattices measured in the US. The one-sigma statistical error for these calculations is about .0002. Once again, the preVII data provides substantial improvements, but the final results for multiplication are still a little lower than experiment.

The Valduc series of experiments is French, and they

TABLE 8. Low-Enriched (2.6wt%) Uranium Oxide and Water Lattices

Assembly Name	**Release 8 k-eff C/E**	**preVII k-eff C/E**
LCT006-1	.9925	.9985
LCT006-2	.9931	.9991
LCT006-3	.9930	.9990
LCT006-6	.9937	.9993
LCT006-7	.9929	.9991
LCT006-8	.9932	.9993
LCT006-9	.9938	.9990
LCT006-10	.9939	.9987
LCT006-11	.9942	.9995
LCT006-12	.9933	.9992
LCT006-13	.9935	.9992
LCT006-14	.9945	.9992
LCT006-15	.9948	.9993
LCT006-16	.9942	.9991
Average	.9936	.9991
Std.Dev.	.0007	.0003

TABLE 9. Low-Enriched (2.35wt%) Uranium Oxide and Water Lattices

Assembly Name	**Release 8 k-eff C/E**	**preVII k-eff C/E**
LCT001-1	.9951	.9992
LCT001-2	.9940	.9976
LCT001-3	.9937	.9974
LCT001-4	.9944	.9985
Average	.9943	.9982

were done with a variety of pin placements in the lattice leading to a wide range of effective lattice pitch values. The enrichment for these pins was 4.74wt%. Table 11 shows that much of the C/E deviation is fixed by the preVII cross sections, but in addition, the bias with pin arrangement is greatly reduced. The results in Table 12 also show some improvement, but as for the other assemblies with higher enrichment values, the average k-eff for this set is still a little low. The MCNP Valduc models were provided by Harish Huria of Westinghouse. These were run to a one-sigma accuracy of about .00025.

The LCT lattice criticals studied above are smaller than real power reactors with fewer rods and higher leakages. They are typically brought to critical by adjusting the water level, so they are inherently three dimensional (making Monte Carlo methods preferred for getting good results). In order to see how the preVII cross sections perform with something more like a real power reactor, we analyzed the Babcock&Wilcox XI-2 core (LCT008 case 2 in the ICSB Handbook) with a large number of uranium oxide rods. This assembly was brought to critical using boron concentration, so it is well behaved for both 2-D and 3-D calculations. The MCNP B&W model was provided by Russ Mosteller of Los Alamos. We also constructed a full 3-D model for the TRX-1 assembly based on CSEWG specifications—this assembly used 764 uranium metal rods with 1.3wt% enrichment and aluminum cladding in a triangular arrangement. A similar model for BAPL-1 has 2173 aluminum-clad uranium-oxide 1.3wt% rods. The results are in Table 13. The one-sigma statistical accuracy was about .0002 for these calculations. Once again, the preVII cross sections perform fairly well.

TABLE 10. Low-Enriched (4.31wt%) Uranium Oxide and Water Lattices

Assembly Name	**Release 8 k-eff C/E**	**preVII k-eff C/E**
LCT002-1	.9938	.9973
LCT002-2	.9920	.9964
LCT002-3	.9941	.9983
LCT002-4	.9932	.9978
Average	.9933	.9973

TABLE 11. Valduc LCT007 Lattices

Assembly Name	**Release 8 k-eff C/E**	**preVII k-eff C/E**
LCT007-1	.9914	.9974
LCT007-2	.9949	.9989
LCT007-4	.9964	.9981
Average	.9942	.9981

TABLE 12. Valduc LCT039 Lattices

Assembly Name	**Release 8 k-eff C/E**	**preVII k-eff C/E**
LCT039-1	.9909	.9964
LCT039-2	.9925	.9975
LCT039-3	.9921	.9968
LCT039-4	.9907	.9959
LCT039-5	.9933	.9978
LCT039-7	.9947	.9966
LCT039-8	.9917	.9966
LCT039-9	.9921	.9963
LCT039-10	.9928	.9988
Average	.9923	.9970

TABLE 13. Large Lattices

Assembly Name	**Release 8 k-eff C/E**	**preVII k-eff C/E**
B&W XI-2	.9977	.9996
TRX-1	.9910	.9971
BAPL-1	.9964	1.0012

CONCLUSIONS

The proposed preVII cross sections show good performance for fast critical assemblies (U233, U235, U238, and Pu239), thermal uranium solution criticals, and thermal lattices of uranium oxide rods. Some additional small adjustments are anticipated before the final release of ENDF/B-VII, but these results suggest that the new library of evaluated nuclear data will be a significant improvement for many important applications.

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