LA-UR 95-1886

CONF-9509100--28

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

TITLE: TESTING OF THE ENDF/B-VI NEUTRON DATA LIBRARY ENDF60 FOR USE WITH MCNP™

AUTHOR(S): S.C. Frankle

SUBMITTED TO: 1995 Nuclear Criticality Technology Safety Project

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO. 836 R4
ST. NO. 2629 5/81

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

TESTING OF THE ENDF/B-VI NEUTRON DATA LIBRARY ENDF60 FOR USE WITH MCNP™

S. C. Frankle and R. E. MacFarlane
Los Alamos National Laboratory

ABSTRACT

The continuous-energy neutron data library ENDF60, for use with the Monte Carlo N-Particle radiation transport code MCNP4A,[1] was released in the fall of 1994. It is comprised of 124 nuclide data files based on the ENDF/B-VI evaluations through Release 2. Forty-eight percent of these materials are new or modified evaluations, while the balance are translations from ENDF/B-V. The new evaluations include most of the important materials for criticality safety calculations, and include significant enhancements such as more isotopic evaluations, better resonance-range representations, and the new correlated energy-angle distributions for emitted particles. As part of the overall quality assurance testing of the ENDF60 library, calculations for well known benchmark assemblies were performed. The results of these calculations help the user to know how the combination of ENDF60 and MCNP4A will perform for real problems.

INTRODUCTION

Accurate calculations of radiation transport and neutron multiplication in systems with complex composition and geometry are common in the criticality safety field. As computer power, user sophistication, and regulatory oversight have advanced, more of these calculations are made using physically detailed methods, such as the Monte Carlo N-Particle transport code MCNP. Highly capable codes like MCNP also require up-to-date nuclear data, such as those contained in the latest version of the US standard Evaluated Nuclear Data Files, ENDF/B-VI.[2] For the criticality safety expert, it is the combination of the transport code and data library that must be proven, and the purpose of this paper is to present results to help in making this judgment.

ENDF/B-VI (B-VI) was first released in 1990. The original release was followed by minor updates in Release 1 in 1991, and by a number of significant improvements in Release 2 in 1993. Fifty-two percent of the evaluations used for the ENDF60 library are translations from ENDF/B-V. The remaining forty-eight percent are new or modified evaluations, which have sometimes changed significantly. Among these changes are a greatly increased use of isotopic evaluations (especially for important structural materials like Fe, Cr, Ni, and Cu), much more sophisticated and extensive resonance-parameter evaluations (such as ^{235}U and ^{238}U), and energy-angle correlated distributions for emitted particles. Fission yield and radioactive decay data have also been hugely expanded. The bulk of B-VI and its many new features have somewhat delayed its usage in the applications community.

The ENDF-format evaluations were processed using the NJOY Nuclear Data Processing System [3] to produce data libraries in the ACE (A Compact ENDF) format used by MCNP. During the period 1989 to 1993, NJOY was gradually updated to handle most of the new features of B-VI. In addition, there was a cooperative effort between the NJOY and MCNP teams to enable MCNP and the ACE format to support these new features. Some of the new features include the addition of three new scattering laws (which also involved new data formats, processing methods, transport physics, and a next-event estimator and point detector sampling scheme). These three laws are the Kalbach-87 energy-angle formalism (ENDF File 6 LAW=1, LANG=2; MCNP law 44), correlated angle-energy distributions (ENDF File 6 LAW=7; MCNP law 67), and the phase-space law (ENDF File 6 LAW=6; MCNP law 66). Extensive tests were carried out to ensure that the new scattering laws were properly implemented in MCNP4A and that both transport and next-event estimator solutions agreed. A more detailed discussion of these laws can be found in reference 4.

This work culminated in the processing of the materials for the ENDF60 library using NJOY in late 1993, the testing of the library with MCNP4A during the summer of 1994, and the release of the ENDF60 library in the fall of 1994 to the Radiation Shielding Information Center at Oak Ridge National Laboratory.

ENDF60 DATA TESTING

A number of new quality assurance tests for the ENDF60 library were implemented by the Nuclear Theory and Applications group (T-2) and the Radiation Transport group (X-6). At the lowest level, these included trials to make sure that the files could be printed, plotted, converted to other forms, and staged into MCNP correctly. Key materials were examined by eye and new features were validated by comparison to hand calculations. Many of these low level tests have now been incorporated into the ACER module of the NJOY code to help other users to be able to generate reliable data libraries. Additionally, integral tests were performed by comparing the ENDF60 library with previously available data libraries for a set of infinite-medium and photon production simulations.[5,6]

These kinds of checks are useful for finding errors in the codes and data sets, but most users are more interested in how the combination of the transport code and the data library will perform for their applications. For this reason, the ENDF60 data library was also compared with experimental benchmarks using the Lawrence Livermore Pulsed Sphere experiments and a set of four iron benchmark experiments.[7,8] Additionally, results from the ENDF60 and the ENDF/B-V (B-V) data libraries were compared for a set of nine benchmark critical assemblies that have been used in the past for testing MCNP and for a set of twenty-five benchmark problems for the KENO code.[9,10] Some of the previous MCNP benchmarks had been simplified, and some of the KENO problems are repeats of one another or fictitious (such as an infinite cylinder). Because of these limitations, these results were useful for seeing how the codes and libraries have changed, but were not necessarily useful for ensuring the accuracy of the computational system. With these caveats, Tables 1 and 2 show the results from both sets of criticality benchmarks using the existing B-V based library and the new ENDF60 library.[4] The column labeled "Recommended" in Table 1 shows the results when the ^{239}Pu in a plutonium assembly is replaced by the recommended evaluation, which was generated for ENDF/B-V.2 and formed the base for the B-VI evaluation.

PERFORMANCE TESTING

For real performance testing, it is important to have a realistic model for the critical assembly. We have revised four of the MCNP models for the assemblies in LA-12212 and defined eight new benchmarks using the specifications from the Cross Section Evaluation Working Group (CSEWG) data testing manual.[11] The remaining five critical assemblies in LA-12212 are still under review. The material specifications for the 3x3 array of Pu fuel rods is known to be correct and the improved B-VI results are thought to be accurate.[9,17] No review of the KENO tests cases has been performed. In the current test suite, there are now four bare critical assemblies; Godiva (CSEWG-F5) [9,11-13] is a bare sphere of highly enriched uranium, Jezebel (CSEWG-F1) [9,11-

13 is a bare sphere of enriched ^{239}Pu, Jezebel-Pu is a bare sphere of 20% ^{240}Pu plutonium (CSEWG-F21) [9,11-13], and Jezebel-23 (CSEWG-F19) [11,12] is a bare sphere of ^{233}U. There are four natural uranium reflected assemblies; Flattop-25 (CSEWG-F22) [11-13] has a core of enriched uranium, Flattop-Pu (CSEWG-F23) [11-13] has a core of Pu-239, Flattop-23 (CSEWG-F24) [11-13] has a core of U-233, and Bigten (CSEWG-F20) [11] is a larger assembly with a 10% U-235 core Additionally, there is also a natural thorium reflected ^{239}Pu sphere benchmark, Thor (CSEWG-F25) [11,12]. There are three thermal benchmarks; ORNL-1 (CSEWG-T1) [11] a large sphere of uranyl nitrate solution , L-7 (proposed CSEWG) [15] a water-reflected sphere of uranyl fluoride solution, and a water-reflected uranium sphere[9,14].

The results for these assemblies are given in Table 3 for both the ENDF/B-V and ENDF/B-VI libraries. The entries for Godiva, Jezebel, Jezebel-Pu, and the water-reflected uranium sphere can be compared to the corresponding entries in Table 2 to see the effects of the revised models. The results for Godiva have decreased and increased for the B-V and B-VI based libraries respectively, with the B-VI library giving a value for k_{eff} closer to 1.0. The results for the plutonium spheres of the Jezebel assemblies have decreased, coming closer to a value of 1.0 for both libraries. The results for the water-reflected uranium sphere remain relatively unchanged for both libraries. Overall, the results for the bare uranium and plutonium spheres are quite good with the B-VI based library ENDF60.

The ^{233}U evaluation was translated from B-V to B-VI, however photon production was added after the MCNP B-V based library was processed. For these benchmarks, the addition of photon production to the evaluation should not affect the results. The primary changes between MCNP libraries for ^{233}U are due to improvements in the processing code NJOY. The results in Table 3 indicate that both libraries give similar results for Jezebel-23 and Flattop-23.

All of the natural uranium reflected assemblies give moderately high results for k_{eff} for both B-V and B-VI. This has been a long-standing feature of CSEWG calculations for these assemblies, and it suggests that some work needs to be done on the transport cross section for ^{238}U. The thorium reflected assembly, Thor, has improved somewhat from B-V to B-VI, however the result is still quite high for B-VI. This has also been a long-standing feature of the CSEWG benchmark, and may indicate a need for a new evaluation of thorium.

The performance of ENDF60 for thermal systems is somewhat more complicated. The results for the water-reflected sphere of uranium were discussed above and remain relatively unchanged. The three cylinders of uranium solution[16] from Table 1 is known to have material specification problems that have not been corrected, and cannot be used to judge the accuracy of ENDF60 at this time. The results from ORNL-1 show a significant decrease, while the results from L-7 remain relatively unchanged. It is difficult to separate out the contribution to the change in k_{eff} as H, O, C, and F are also all new evaluations. Simulations performed using the B-V evaluation for ^{235}U with all other nuclides specified as B-VI gave values for k_{eff} of 0.9907 ± 0.0016, 0.9963 ± 0.0009, and 1.0007 ± 0.0019 for the water-reflected uranium sphere, ORNL-1 and L-7 benchmarks respectively. This indicates a decrease, sometimes very small, in k_{eff} for most of the B-V and B-VI results. This seems to indicate that the B-VI evaluation for ^{235}U is more reactive, giving higher values for k_{eff}.

In the past, the CSEWG thermal data testing effort has obtained interesting results for the series of large homogeneous uranyl-nitrate solution assemblies (ORNL-1 and others) and for a series of smaller uranyl-fluoride assemblies (L-7 and others), both built at ORNL. Earlier B-V and B-VI multigroup calculations show a trend of increasing multiplication with increasing leakage (typically 0.6 to 0.7 percent between the low leakage and high leakage limits).[18] In addition, the multiplication for the low-leakage systems with B-VI gave low values for k_{eff} by approximately 0.3 percent, with B-V values being very close to unity. An analysis of the situation suggested that the resonance capture integral for ^{235}U was the source of the leakage bias and small problems in the thermal cross sections were responsible for the low multiplication. A modified evaluation is being prepared for Release 3 of ENDF/B-VI.[19]

CONCLUSIONS

The combination of MCNP4A and the ENDF60 library is now available for making criticality safety calculations. The combination of the geometrical flexibility, faithful physics modeling, and continuous-energy accuracy of MCNP with the modern cross section data of ENDF60 provides a very powerful and defendable tool. The new library gives quite good results for a variety of critical assemblies, and the new data which will become available from Release 3 of B-VI will hopefully improve the performance of the system even more in the near future.

REFERENCES

1 "MCNP-A General Monte Carlo N-Particle Transport Code", ed. J. Briesmeister Los Alamos National Laboratory manual, LA-12625 (1993).

2 "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6", ed. P. Rose and C. Dunford, Brookhaven National Laboratory, BNL-NCS-44945 (revised 1991).

3 R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91," Los Alamos National Laboratory manual LA-12740-M (1994).

4 "ENDF/B-VI Data for MCNP", J. Hendricks, S. Frankle, and J. Court, Los Alamos National Laboratory Report, LA-12891 (1994).

5 "MCNP ENDF/B-VI Validation: Infinite Media Comparisons of ENDF/B-VI and ENDF/B-V", J. Court, J. Hendricks, and S. Frankle, Los Alamos National Laboratory Report, LA-12887 (1994).

6 "Photon Production Assessment for the MCNP Data Libraries", S. C. Frankle, Los Alamos National Laboratory report, to be published.

7 "Lawrence Livermore Pulsed Sphere Benchmark Analysis of MCNP ENDF/B-VI", J. Court, R. Brockhoff, and J. Hendricks, Los Alamos National Laboratory Report, LA-12885 (1994).

8 "Benchmark Analysis of MCNP ENDF/B-VI Iron", J. Court and J. Hendricks, Los Alamos National Laboratory Report, LA-12884 (1994).

9 "MCNP: Criticality Safety Benchmark Problems", J. Wagner, J. Sisolak, and G. McKinney, Los Alamos National Laboratory report, LA-12415 (1992).

10 "MCNP: Neutron Benchmark Problems", D. Whalen et al, Los Alamos National Laboratory Report, LA-12212 (1991).

11 "ENDF-202: Cross Section Evaluation Working Group Benchmark Specifications", Brookhaven National Laboratory Report, BNL 19302, (revised 1991).

12 "Los Alamos Critical-Mass Data", H.C. Paxton, Los Alamos National Laboratory report, LA-3067-MS, Rev., (1975).

13 "Reevaluated Critical Specifications of Some Los Alamos Fast-Neutron Systems", G.E. Hansen and H.C. Paxton, Los Alamos National Laboratory report, LA-4208. (1969).

14 "Critical Measurements of a Water-Reflected Enriched Uranium Sphere", C.C. Byers et al., Transactions of the American Nuclear Society, 27, pg. 412 (1977).

15 "Thermal Data Testing Memorandum 81-2", P. Rose, Brookhaven National Laboratory memorandum (1981).
16 "Critical Dimensions of Systems Containing 235U, 239Pu, and 233U", H.C. Paxton and N.L. Pruvost, Los Alamos National Laboratory Report, LA-10860-MS, 1986 Revision, pg. 131 (1987).
17 "Summary of Experimentally Determined Plutonium Array Critical Configurations", H.F. Finn et al., Lawrence Livermore National Laboratory Report, UCRL-51041 (1971).
18 "Data Testing of ENDF/B-VI", R. E. MacFarlane, Proceedings of the International Conference on Nuclear Data for Science and Technology , pg. 786 (1994).
19 "A Modification to ENDF6 U235 To Increase Epithermal Alpha and K1", C. R. Lubitz, Proceedings of the International Conference on Nuclear Data for Science and Technology, pg. 646 (1994).

Table 1: Critical Assembly Benchmarks

	Recommended	ENDF/B-V	ENDF/B-VI
Godiva 93.71% Enriched Bare Sphere	*	1.0001 ± 0.0010	0.9952 ± 0.0011
Jezebel - 95.5% Enriched ^{239}Pu	0.9986 ± 0.0021	1.0151 ± 0.0022	1.0023 ± 0.0022
Jezebel - 80% Enriched ^{239}Pu	1.0080 ± 0.0012	1.0160 ± 0.0012	1.0097 ± 0.0012
Uranium Cylinder 10.9% Enriched ^{235}U	*	1.0010 ± 0.0006	0.9998 ± 0.0005
Uranium Cylinder 14.11% Enriched ^{235}U	*	1.0009 ± 0.0006	0.9972 ± 0.0005
Graphite-Tamped Uranium Sphere	*	0.9869 ± 0.0010	0.9810 ± 0.0010
Water-Reflected Uranium Sphere	*	0.9967 ± 0.0019	0.9961 ± 0.0019
Three Cylinders of Uranium Solution	*	1.0016 ± 0.0013	0.9961 ± 0.0014
3x3 Array of Pu Fuel Rods	1.0008 ± 0.0017	1.0076 ± 0.0017	0.9992 ± 0.0015

Table 2: KENO Benchmarks

	ENDF/B-V	ENDF/B-VI
Keno 1	0.9999 ± 0.0009	0.9936 ± 0.0009
Keno 2	0.9999 ± 0.0009	0.9936 ± 0.0009
Keno 3	0.9993 ± 0.0011	1.0002 ± 0.0011
Keno 4	1.0008 ± 0.0028	0.9998 ± 0.0026
Keno 5	1.0004 ± 0.0028	1.0044 ± 0.0029
Keno 6	0.7461 ± 0.0007	0.7426 ± 0.0007
Keno 7	1.0002 ± 0.0008	0.9954 ± 0.0008
Keno 8	0.9404 ± 0.0008	0.9381 ± 0.0007
Keno 9	2.2910 ± 0.0010	2.2597 ± 0.0009
Keno 10	0.9999 ± 0.0009	0.9936 ± 0.0009
Keno 11	0.9999 ± 0.0009	0.9936 ± 0.0009
Keno 12	0.9987 ± 0.0012	0.9994 ± 0.0013
Keno 13	0.9949 ± 0.0008	0.9914 ± 0.0008
Keno 14	0.9985 ± 0.0008	0.9969 ± 0.0008
Keno 15	1.0016 ± 0.0010	1.0003 ± 0.0011
Keno 16	0.9907 ± 0.0009	0.9924 ± 0.0009
Keno 17	1.0029 ± 0.0014	0.9986 ± 0.0015
Keno 18	1.0280 ± 0.0013	1.0308 ± 0.0013
Keno 19	0.9987 ± 0.0012	0.9994 ± 0.0013
Keno 20	0.9971 ± 0.0013	0.9981 ± 0.0015
Keno 21	0.9951 ± 0.0008	0.9929 ± 0.0009
Keno 22	0.9978 ± 0.0008	0.9955 ± 0.0008
Keno 23	0.9999 ± 0.0009	0.9936 ± 0.0009
Keno 24	0.9982 ± 0.0008	0.9944 ± 0.0008
Keno 25	1.0012 ± 0.0009	0.9952 ± 0.0009

Table 3: Revised and New Criticality Benchmarks for MCNP

	ENDF/B-V	ENDF/B-VI
Godiva CSEWG-F5	0.9953 ± 0.0011	0.9992 ± 0.0012
Jezebel CSEWG-F1	1.0051 ± 0.0018	1.0003 ± 0.0020
Jezebel-Pu CSEWG-F21	1.0041 ± 0.0011	1.0003 ± 0.0012
Jezebel-23 CSEWG-F19	0.9923 ± 0.0011	0.9926 ± 0.0010
Flattop-25 CSEWG-F22	1.0058 ± 0.0015	1.0048 ± 0.0013
Flattop-Pu CSEWG-F23	1.0088 ± 0.0015	1.0042 ± 0.0015
Flattop-23 CSEWG-F24	1.0031 ± 0.0015	1.0041 ± 0.0015
Bigten -2D CSEWG-F20	1.0031 ± 0.0010	1.0053 ± 0.0011
Thor CSEWG-F25	1.0138 ± 0.0014	1.0083 ± 0.0013
Water-Reflected Uranium Sphere	0.9967 ± 0.0019	0.9946 ± 0.0018
ORNL-1 CSEWG-T1	1.0007 ± 0.0010	0.9956 ± 0.0009
L-7 Proposed CSEWG	1.0034 ± 0.0017	1.0022 ± 0.0016