Title: Release of ENDF/B-VII.1-based Continuous Energy Neutron Cross Section Data Tables for MCNP

Author(s): Conlin, Jeremy Lloyd
Gardiner, Steven J.
Parsons, Donald K.
Kahler, Albert C. III
Lee, Mary Beth
White, Morgan C.

Intended for: 2013 ANS Annual Meeting, 2013-06-16 (Atlanta, Georgia, United States)
INTRODUCTION

In December 2011, the National Nuclear Data Center (NNDC) released ENDF/B-VII.1 [1], the “latest recommended evaluated nuclear data file for use in nuclear science and technology applications”. The data was released in the standard Evaluated Nuclear Data Format (ENDF-6) [2]. This release represents the advances made in nuclear data during the five years since the release of ENDF/B-VII.0 [3].

The ENDF/B-VII.1 library consists of all of the evaluations included in the ENDF/B-VII.1 neutron evaluation files and has made available a library of ACE data tables at several temperatures for each of the ENDF/B files. The data was processed with the NJOY code, version 99.393, except for 35Cl which was processed with NJOY version 2012.0b. The ACE data library is called ENDF71x and has been distributed through RSICC along with MCNP6.

The ENDF71x library consists of all of the evaluations included in the ENDF/B-VII.1 library processed at the same five temperatures that were used in the ENDF/B-VII.0-based release of ACE data [4] as well as two lower temperatures, 0.1 K and 250 K, for use in creating on-the-fly Doppler broadened cross sections [5]. Table I lists all seven temperatures that is available in the ENDF71x library.

<table>
<thead>
<tr>
<th>ZA Suffix</th>
<th>SZA Extensions</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>80c</td>
<td>710nc</td>
<td>293.6 K</td>
</tr>
<tr>
<td>81c</td>
<td>711nc</td>
<td>600 K</td>
</tr>
<tr>
<td>82c</td>
<td>712nc</td>
<td>900 K</td>
</tr>
<tr>
<td>83c</td>
<td>713nc</td>
<td>1200 K</td>
</tr>
<tr>
<td>84c</td>
<td>714nc</td>
<td>2500 K</td>
</tr>
<tr>
<td>85c</td>
<td>715nc</td>
<td>0.1 K</td>
</tr>
<tr>
<td>86c</td>
<td>716nc</td>
<td>250 K</td>
</tr>
</tbody>
</table>

TABLE I. Suffixes and temperatures for the nuclide identifier.

The ENDF/B-VII.1 library contains evaluations for 423 nuclides. Two evaluations were removed in ENDF/B-VII.1; the elemental evaluations for vanadium and zinc. They were replaced with isotopic evaluations for the same elements. A total of 32 new evaluations were added in ENDF/B-VII.1; one of them, 254m1Es, was a metastable evaluation, the rest are ground state evaluations. A list of all the added evaluations in ENDF/B-VII.1 are given here

1. 50V  9. 168Tm  17. 229Pa  25. 246Bk
2. 51V  10. 169Tm  18. 230Pa  26. 247Bk
3. 64Zn 11. 170Tm  19. 230U  27. 248Bk
4. 65Zn 12. 180Tm  20. 231U  28. 246Cf
5. 66Zn 13. 180W  21. 234Np  29. 248Cf
6. 67Zn 14. 203Tl  22. 240Am  30. 251Es
7. 68Zn 15. 205Tl  23. 240Cm  31. 252Es
8. 70Zn 16. 231Th  24. 245Bk  32. 254m1Es

With new additions the xsdir file, which contains atomic weight ratios for all the nuclides for which there is data referenced in the file, required an update. The atomic weight ratios were updated using the weight ratios documented in reports by Audi, Wapstra, and Thibault [6].

This summary serves to make known the availability of the ENDF71x library. There is not sufficient space here to document all the features and characteristics of the library. A user of the library is strongly encouraged to consult the official documentation [7] accompanying the data release.

IDENTIFYING ENDF71x DATA TABLES

Each of the 423 ENDF/B-VII.1 evaluations were processed at each of the seven temperatures making 2961 ACE data tables in the ENDF71x library. Each ACE data table can be identified by a unique identifier specified by the atomic number, Z, and the atomic mass number, A, and a suffix or extension. The ZAID combined with the suffix constitutes a ZAID.

The ENDF71x library can use the traditional ZAID format to identify the ACE data tables, or the new SZAX format (defined in reference [8])—if supported by the transport code. The ZAs associated with the ENDF71x library are listed in Table II.

The ZA suffixes and SZA extensions used to identify the ACE data tables in the ENDF71x library are 8tc and 71tnc, respectively, where t ranges from 0–6 and refers to the temperatures to which the evaluations were processed; 293.6 K, 600 K, 900 K, 1200 K, 2500 K, 0.1 K and 250 K respectively. Table II shows the SUA suffix and SZA extension for the different temperatures available in the ENDF71x library. The ZA along with suffix make up a unique ZAID used to identify an ACE data table.

With the first production release of MCNP6 there will be no support for the SZA identifiers; support for SZAX is planned for subsequent releases of MCNP6. Until the SZAX identifiers are supported, care must be taken to ensure that the correct ACE data table is used. Unexpected results will occur when using SZA identifiers in a code that doesn’t support them.
TABLE II. List of ZAs for the ACE data tables released with ENDF71x. The separations are merely for convenience and show the light (Z < 25), mid-weight (25 ≤ Z < 89) and the actinides. The ZAIDs with an asterisk (*) indicate evaluations new to ENDF/B-VII.1 and ZAIDs new in the ENDF71x library.
TESTING AND WARNINGS

The ENDF71x library has been the most heavily tested ACE library released by the Nuclear Data Team at LANL. We have run a suite of internal checking programs to verify the integrity of the data and we have mechanically run every new ACE data table in MCNP5 and MCNP6. Finally we plotted and visually inspected six important quantities for every ACE data table. A full description of what was checked can be found in the full documentation for the ENDF71x library [7]; short descriptions are given in the following sections.

Our testing revealed a number of features in the data that are summarized below. All of the problems mentioned here originate from the ENDF/B-VII.1 evaluations; none of them is due to the processing of the data.

checkace

A suite of programs developed for internal use at LANL was run. This suite is referred to as checkace and consists of a number of separate programs that read the ACE data table and verifies various formats and physics.

Using the checkace suite of programs, we discovered that the ENDF/B evaluation for $^{153}$Eu contains probability distribution functions (PDFs) with negative values. checkace replaced the negative values with 0.0, renormalized the distribution, and rewrote the ACE data table. The ACE data table is fine, but doesn’t perfectly reflect what was intended in the ENDF/B-VII.1. All of the evaluations that we have found with energy balance issues were flagged by MacFarlane. Listed here are the evaluations that checkace found having negative heating values.

1. $^{33}$S
2. $^{36}$S
3. $^{99}$Zr
4. $^{92}$Zr
5. $^{93}$Zr
6. $^{94}$Zr
7. $^{95}$Zr
8. $^{96}$Zr
9. $^{93}$Nb
10. $^{92}$Mo
11. $^{94}$Mo
12. $^{90}$Mo
23. $^{151}$Sm
24. $^{153}$Gd
25. $^{153}$Gd
26. $^{115m}$Cd
27. $^{165}$Ho
28. $^{166}$Er
29. $^{168}$Tm
30. $^{145}$Nd
31. $^{147}$Nd
32. $^{147}$Sm
33. $^{148}$Sm
34. $^{179}$Hf
35. $^{180}$Hf
36. $^{197}$Au
37. $^{196}$Hg
38. $^{202}$Hg
39. $^{203}$Tl
40. $^{205}$Tl
41. $^{209}$Bi

Negative heating values may cause problems with energy deposition or kerma calculations. We don’t anticipate the problems with the negative heating values in ENDF71x to drastically alter calculations, but the user should be aware of the problems.

There appears to be problems with the unresolved resonance range in the following evaluations:

1. $^{22}$Na 5. $^{70}$Ge 9. $^{186}$W 13. $^{249}$Bk
2. $^{36}$Ar 6. $^{106}$Cd 10. $^{203}$Tl 14. $^{249}$Cf
3. $^{58}$Co 7. $^{170}$Tm 11. $^{232}$U 15. $^{250}$Cf
4. $^{65}$Zn 8. $^{182}$W 12. $^{236}$Pu

These evaluations generated a number of errors in checkace indicating that the sum of the partial cross sections did not equal the total cross section in the unresolved resonance region. These evaluations were reprocessed with NJOY without using the PURR module. When an ACE file is created without running the PURR module, the cross section values in the unresolved resonance range are the average cross sections provided in the MF=3 section of the ENDF/B file.

Mechanical Testing

An heroic effort was performed by Gardiner et al. in testing each of the 2961 ACE data tables in MCNP5 and MCNP6. Each ACE data table was used in several calculations designed to exercise as much of the data table as possible. The full report of this work is found in the M&C conference paper [10].

There were a few times where new and expanded data has caused MCNP to crash. These problems are fixed in MCNP6, but those using the ENDF71x data with MCNP5 should be aware of the potential for the code to crash.

The isotopes $^{231,233}$Pa have bad data in that the number of secondary neutrons from MT=5 is much too large. MCNP5 has a limit of 11 secondary neutrons—if more than 11 secondary neutrons are produced then problems occur in array accessing that cause MCNP to crash due to a segmentation fault. The physical number of secondary neutrons is not new to ENDF/B-VII.1, it also existed in ENDF/B-VII.0.

Another issue with the data and older versions of MCNP (i.e., < MCNP6) occurs when a continuum distribution of secondary gammas is not defined for every incident energy for threshold reactions. When this data is encountered, arrays are accessed beyond their bounds and MCNP eventually crashes due to a segmentation fault. This is a very rare occurrence—it was only observed by (un)lucky chance in $^{226}$Ac in an (n, 4n) reaction—but could potentially happen with the following nuclides:

1. $^{226}$Ac
2. $^{227}$Th
3. $^{228}$Th
4. $^{230}$Th
5. $^{233}$Th
6. $^{234}$Th
7. $^{236}$Pa
8. $^{232}$U
9. $^{235}$Np
10. $^{224}$Pu
11. $^{226}$Pu
12. $^{243}$Pu
13. $^{245}$Cm
14. $^{246}$Cm
15. $^{248}$Cm
16. $^{249}$Cm
17. $^{242}$Pu
18. $^{246}$Pu
19. $^{249}$Pu
20. $^{246}$Cm
21. $^{250}$Cm
22. $^{251}$Cf
23. $^{252}$Cf
24. $^{253}$Cf
25. $^{254}$Cf
26. $^{252}$Es
27. $^{253}$Es
28. $^{255}$Es
**Visual Inspection**

We have performed a visual inspection of the room temperature cross sections for these reactions: 1) total, 2) absorption, 3) elastic scattering, 4) total fission, 5) \((n, 2n)\), and 6) average heating number. Plotting and visually inspecting the cross sections can spot errors that our other checking methods have not found.

Two unusual and unphysical features were obvious from our inspection: 1) gaps in the heating number and 2) "sawtooth" cross sections. Gaps in the heating number occur because of the negative heating numbers discussed previously. The evaluations with sawtooth patterns here because it is not a fundamental problem with the data. The evaluations with sawtooth problems are listed in the formal documentation.

Many evaluations (62) had unphysical features we refer to as "sawtooth" patterns. A sawtooth pattern occurs where there is a sudden change in the cross section of several orders of magnitude--and is not a resonance. The cause of these sawtooth patterns are due to the process in which the evaluation was tabulated in the ENDF/B file. We do not list the evaluations that had sawtooth patterns here because it is not a fundamental problem with the data. The evaluations with sawtooth problems are listed in the formal documentation.

**CONCLUSION**

The release of the ENDF71x library represents five years of work updating ENDF/B-VII.0 to ENDF/B-VII.1 followed by a full years worth of work by the Nuclear Data Team at LANL. The library was processed from ENDF/B-VII.1 evaluations into ACE data tables using NJOY 99.393 for seven temperatures.

The ENDF71x library has been heavily tested and verified. The ENDF71x library is recommended for use in all Monte Carlo applications with the caveats detailed in this summary and in the complete documentation [7].

**REFERENCES**


