LA-UR-13-20240
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Intended for: 2013 ANS Annual Meeting, 2013-06-16 (Atlanta, Georgia, United States)

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

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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 Nuclear Data Team at Los Alamos National Laboratory (LANL) has processed the entire 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 ^{35}Cl 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.

ZA Suffix	SZA eXtension	Temperature
80c	710nc	293.6 K
81c	711nc	600 K
82c	712nc	900 K
83c	713nc	1200 K
84c	714nc	2500 K
85c	715nc	0.1 K
86c	716nc	250 K

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, ^{254m1}Es, 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. ^{50}V
2. ^{51}V
3. ^{64}Zn
4. ^{65}Zn
5. ^{66}Zn
6. ^{67}Zn
7. ^{68}Zn
8. ^{70}Zn
9. ^{168}Tm
10. ^{169}Tm
11. ^{170}Tm
12. ^{180}Ta
13. ^{180}W
14. ^{203}Tl
15. ^{205}Tl
16. ^{231}Th
17. ^{229}Pa
18. ^{230}Pa
19. ^{230}U
20. ^{231}U
21. ^{234}Np
22. ^{240}Am
23. ^{240}Cm
24. ^{245}Bk
25. ^{246}Bk
26. ^{247}Bk
27. ^{248}Bk
28. ^{246}Cf
29. ^{248}Cf
30. ^{251}Es
31. ^{252}Es
32. ^{254m1}Es

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 ZA 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 I shows the ZA 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 SZAX 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 SZAX identifiers in a code that doesn't support them.

1001	1002	1003	2003	2004	3006	3007	4007	4009	5010
5011	6000	7014	7015	8016	8017	9019	11022	11023	12024
12025	12026	13027	14028	14029	14030	15031	16032	16033	16034
16036	17035	17037	18036	18038	18040	19039	19040	19041	20040
20042	20043	20044	20046	20048	21045	22046	22047	22048	22049
22050	23050*	23051*	24050	24052	24053	24054	25055		
26054	26056	26057	26058	27058	27059	27458	28058	28059	28060
28061	28062	28064	29063	29065	30064*	30065*	30066*	30067*	30068*
30070*	31069	31071	32070	32072	32073	32074	32076	33074	33075
34074	34076	34077	34078	34079	34080	34082	35079	35081	36078
36080	36082	36083	36084	36085	36086	37085	37086	37087	38084
38086	38087	38088	38089	38090	39089	39090	39091	40090	40091
40092	40093	40094	40095	40096	41093	41094	41095	42092	42094
42095	42096	42097	42098	42099	42100	43099	44096	44098	44099
44100	44101	44102	44103	44104	44105	44106	45103	45105	46102
46104	46105	46106	46107	46108	46110	47107	47109	47111	47610
48106	48108	48110	48111	48112	48113	48114	48116	48515	49113
49115	50112	50113	50114	50115	50116	50117	50118	50119	50120
50122	50123	50124	50125	50126	51121	51123	51124	51125	51126
52120	52122	52123	52124	52125	52126	52128	52130	52132	52529
52627	53127	53129	53130	53131	53135	54123	54124	54126	54128
54129	54130	54131	54132	54133	54134	54135	54136	55133	55134
55135	55136	55137	56130	56132	56133	56134	56135	56136	56137
56138	56140	57138	57139	57140	58136	58138	58139	58140	58141
58142	58143	58144	59141	59142	59143	60142	60143	60144	60145
60146	60147	60148	60150	61147	61148	61149	61151	61648	62144
62147	62148	62149	62150	62151	62152	62153	62154	63151	63152
63153	63154	63155	63156	63157	64152	64153	64154	64155	64156
64157	64158	64160	65159	65160	66156	66158	66160	66161	66162
66163	66164	67165	67566	68162	68164	68166	68167	68168	68170
69168*	69169*	69170*	71175	71176	72174	72176	72177	72178	72179
72180	73180*	73181	73182	74180*	74182	74183	74184	74186	75185
75187	77191	77193	79197	80196	80198	80199	80200	80201	80202
80204	81203*	81205*	82204	82206	82207	82208	83209	88223	88224
88225	88226								
89225	89226	89227	90227	90228	90229	90230	90231*	90232	90233
90234	91229*	91230*	91231	91232	91233	92230*	92231*	92232	92233
92234	92235	92236	92237	92238	92239	92240	92241	93234*	93235
93236	93237	93238	93239	94236	94237	94238	94239	94240	94241
94242	94243	94244	94246	95240*	95241	95242	95243	95244	95642
95644	96240*	96241	96242	96243	96244	96245	96246	96247	96248
96249	96250	97245*	97246*	97247*	97248*	97249	97250	98246*	98248*
98249	98250	98251	98252	98253	98254	99251*	99252*	99253	99254
99255	99754*	100255							

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 ($25 \leq Z < 89$) 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 reveled 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 evaluation—but we feel that our ACE data table is a slight improvement.

There were a combined 8624 negative heating values in 41 evaluations. MacFarlane [9], on his website http://t2.lanl.gov/data/endf/ebalVII.1/summary.html, has a lengthy description of the energy balance (including heating problems) issues involved with ENDF/B-VII.1. All of the evaluations that we have found with energy balance issues were also flagged by MacFarlane. Listed here are the evaluations that checkace found having negative heating values.

1. ^{33}S
2. ^{36}S
3. ^{59}Ni
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. ^{96}Mo
13. ^{97}Mo
14. ^{98}Mo
15. ^{115m1}Cd
16. ^{132}Te
17. ^{529}Te
18. ^{143}Ce
19. ^{145}Nd
20. ^{147}Nd
21. ^{147}Sm
22. ^{149}Sm
23. ^{151}Sm
24. ^{153}Gd
25. ^{155}Gd
26. ^{165}Ho
27. ^{566}Ho
28. ^{166}Er
29. ^{168}Tm
30. ^{174}Hf
31. ^{176}Hf
32. ^{177}Hf
33. ^{178}Hf
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
2. ^{36}Ar
3. ^{58}Co
4. ^{65}Zn
5. ^{70}Ge
6. ^{106}Cd
7. ^{170}Tm
8. ^{182}W
9. ^{186}W
10. ^{203}Tl
11. ^{232}U
12. ^{236}Pu
13. ^{249}Bk
14. ^{249}Cf
15. ^{250}Cf.

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 MCNP5 to crash due to a segmentation fault. The unphysical 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. ^{230}Pa
8. ^{232}U
9. ^{235}Np
10. ^{242}Pu
11. ^{246}Pu
12. ^{243}Cm
13. ^{245}Cm
14. ^{247}Cm
15. ^{248}Cm
16. ^{249}Cm
17. ^{246}Bk
18. ^{248}Bk
19. ^{249}Bk
20. ^{246}Cf
21. ^{250}Cf
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 were present in 37 evaluations. The gaps in the plot of the heating number occur because of the negative heating numbers discussed previously. The evaluations that had gaps in the heating number are listed here.

1. ^{33}S
2. ^{36}S
3. ^{39}K
4. ^{59}Ni
5. ^{92}Zr
6. ^{93}Zr
7. ^{94}Zr
8. ^{95}Zr
9. ^{96}Zr
10. ^{93}Nb
11. ^{92}Mo
12. ^{94}Mo
13. ^{96}Mo
14. ^{97}Mo
15. ^{98}Mo
16. ^{115m1}Cd
17. ^{132}Te
18. ^{143}Ce
19. ^{147}Sm
20. ^{149}Sm
21. ^{151}Sm
22. ^{166m1}Ho
23. ^{166}Er
24. ^{168}Tm
25. ^{174}Hf
26. ^{176}Hf
27. ^{177}Hf
28. ^{178}Hf
29. ^{179}Hf
30. ^{180}Hf
31. ^{197}Au
32. ^{196}Hg
33. ^{199}Hg
34. ^{202}Hg
35. ^{203}Tl
36. ^{205}Tl
37. ^{209}Bi

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].

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