

LA-UR-13-20137

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Intended for: Report



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Continuous Energy Neutron Cross Section Data Tables Based upon ENDF/B-VII.1

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February 14, 2013

Contents

1	Introduction	2
1.1	ZA Identifiers	2
1.2	SZAX Identifiers	3
1.3	Changes in ENDF/B-VII.1 Since ENDF/B-VII.0	7
1.4	Modifications to ENDF/B-VII.1 in ENDF71x	8
2	Warnings and Issues	8
3	Testing	10
3.1	Verification of Data with checkace	11
3.2	Validation through Mechanical Testing With MCNP6 and MCNP5	15
3.2.1	Crashes of MCNP Encountered During Mechanical Testing	15
3.3	Visual Inspection of Major Cross Sections	17
A	Typical NJOY Input Deck	24
B	MCNP Input File For Testing	25

Abstract

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) [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 has processed the ENDF/B-VII.1 library and has made available a library of ACE data tables at several temperatures for each of the ENDF/B files. The ACE data library is called ENDF71x.

1 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) [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 has processed the ENDF/B-VII.1 library 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 [4], version 99.393. The lone exception is ^{35}Cl which was processed with NJOY version 2012. (An NJOY input deck similar to what we used is shown in Appendix A.) The ACE data library is called ENDF71x and has been distributed through RSICC along with MCNP6.

In 2008, the Nuclear Data Team at Los Alamos National Laboratory released an ACE library based upon ENDF/B-VII.0 [5]. The ENDF/B-VII.0 data files were processed with NJOY version 99.248 for five temperatures; 293.6 K, 600 K, 900 K, 1200 K and 2500 K. The data was made publicly available with the release of MCNP5 version 1.50. The ZAID suffixes associated with this data are 7xc with x ranging from 0–4, corresponding to the temperature of the ACE data table.

The release of the ENDF71x ACE data library includes all the ENDF/B-VII.1 evaluations processed at seven temperatures; the same five temperatures as in the ENDF/B-VII.0-based ACE library as well as 0.1 K and 250 K which are used for on-the-fly Doppler broadening [6]. The ENDF/B-VII.1 library contains evaluations for 423 nuclides. These, evaluated at seven temperatures each, provide 2961 ACE data tables.

1.1 ZA Identifiers

The nuclides in an ACE table are identified by their ZA plus an extension. The ZA plus the extension make up the ZA identifier or ZAID. The current ACE table format allows ten characters for a ZA and a suffix (ID); six digits indicating the ZA, a period, and a two-digit, one-character suffix. The ZAID looks like

$$\text{ZZZAAA.ddC}; \tag{1}$$

where

- ZZZ the atomic number,
- AAA the atomic mass number,
- dd the library identifier,
- T table type.

Note that ZZZ is blank padded, not zero padded if the atomic number is less than 100; e.g., $\text{ZZZ} = 92 \neq 092$ for uranium.

The formula for calculating the ZA for a particular nuclide is:

$$\text{ZA} = 1000 * \text{Z} + \text{A}, \tag{2}$$

where Z is the atomic number and A is the atomic mass number.

The formula for constructing the ZA, as given in Equation (2) has no way of indicating how to pick an evaluation based upon an excited state of an isotope. For excited state evaluations, we chose to follow the ZA construction used in the release of the ENDF/B-VII.0-based, ACE data tables [5]. For excited state evaluations, the formula for constructing a ZA is

$$ZA = 1000 * Z + 300 + s * 100 + A, \quad (3)$$

where s is the excited *state* of the evaluated isotopes; $s = 0$ for the ground state, $s = 1$ for the first excited state, etc. As an example, the ground and excited state ZAs are

27058.80c	ground state
27458.80c	first excited state

A historical exception to the ZA construction formulae given in Equations (2) and (3) is ^{242}Am . For many years, the first excited state for ^{242}Am was the only available evaluation¹ and 95242 was used to identify it. The ground state evaluation was first made available in ENDF/B-VII.0. In order to maintain backwards compatibility, 95242 refers to the first excited state evaluation for ^{242}Am and 95642 refers to the ground state evaluation—the reverse of the convention.

1.2 SZAX Identifiers

With the release of the ENDF/B-VII.1-based ACE data tables (2961 of them), the number of ACE data tables that ship with MCNP is nearly 10 600; more than half of them are incident neutron, continuous-energy data tables. Each data table must be uniquely identified. The number of available ZAID suffixes is diminishing. Because of the near exhaustion of ZAID suffixes, a change in the ZAID format is necessary to expand the number of unique identifiers available.

The Nuclear Data Team along with the MCNP and NJOY teams from LANL have developed a modified identifier for ACE data tables which addresses the near exhaustion of ZAID extensions as well as providing an intuitive way to include excited state information in the identifier. The new identifier and the resulting modification to the ACE table header have been documented [8, 9]. The details will not be recounted here, but the definition of the new identifier is included.

The new formula for creating a unique identifier for a particular data table looks similar to the currently used ZAID;

$$SSZZZAAA.dddCC, \quad (4)$$

where

- SSS the excited state,
- ZZZ the atomic number,
- AAA the atomic mass number,
- ddd the library identifier,
- TT table type.

¹The first excited state has a half-life of 141 yr while the ground state has a half-life of 16.02 h [7].

Like ZZZ, SSS is blank padded and not zero padded.

With the formula in Equation (4), the ground state evaluation keeps the traditional ZA and only the excited state evaluations have a new identifier. Note that since the excited state is now included, the name ZA is incomplete; we will refer to the new identifier as the SZA of the data table and SZAX when referring to the SZA and suffixX as an extended version of the historic use of ZAID².

The new SZA can be constructed using the formula

$$\text{SZA} = \text{S} * 1\,000\,000 + \text{Z} * 1000 + \text{A}. \quad (5)$$

In addition to including the excited state as part of the SZAX, multiple characters can now be used in the suffix to indicate the class of data. For example: incident neutron, continuous energy data, will use the characters nc. Continuing to use ⁵⁸Co as an example, the new SZAX would be

27058.710nc	ground state
1027058.710nc	excited state

ENDF71x ships with both the SZAX and ZAID style of identifying specific libraries. The ZA identifiers for the nuclides included in ENDF71x are given in Table 3. Table 2 shows the ZAs and SZAs for the excited state tables. (For ground state evaluations, the ZA and the SZAX are identical.)

The ZA suffixes for the ENDF71x are 8xc and the SZA extensions are 71xnc where x 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. Note, now there are three digits for the library identifier in the SZAX when there was just two in the ZAID. The ZA and SZA suffixes and their associated temperatures are shown in Table 1.

Warning. MCNP5 and MCNPX do not—and will not—understand a SZAX. In all of the beta releases and at least the first production version of MCNP6 will also not be able to properly handle a SZAX. Future versions of MCNP6 will be able to understand and properly use a SZAX instead of a ZAID.

For those versions of MCNP that can't use a SZAX, problems can arise if a SZAX is specified instead of a ZAID. If a user enters 92235.710nc (hoping for ENDF/B-VII.1-based, room temperature ²³⁵U), the code will not crash, but will use 92235.71c (ENDF/B-VII.0-based, 600 K ²³⁵U) instead. The SZAX entries will be the last ones in the xsdir file and so are only found when the full SZAX is specified. Please make sure that what MCNP uses for its data is what you desired.

²As mentioned previously, ²⁴²Am will continue to be the anomaly with the SZA naming. The ground-state SZA will be 1095242 while the first excited-state will have an SZA of 95242.

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 1: Suffixes and temperatures for the nuclide identifier.

ZA	SZA
27458	1027058
47610	1047110
48515	1048115
52627	1052127
52529	1052129
61648	1061148
67566	1067166
95642	1095242*
95242	95242†
95644	1095244
99754	1099254

Table 2: ZA and SZA identifiers for the isotopes with excited-state data tables.

* ground state of ^{242}Am

† first excited state of ^{242}Am

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	47510
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
52527	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	61548	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	99654*	100255							

Table 3: 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 ZAs with an asterisk (*) indicate isotopes new to ENDF/B-VII.1 and ZAs new in the ENDF71x library.

1.3 Changes in ENDF/B-VII.1 Since ENDF/B-VII.0

The ENDF/B-VII.1 paper by Chadwick et al. [1] states that the ENDF/B-VII.1 library contains advances in nine specific areas. For this paper the relevant advances are:

1. An increase in the breadth of neutron reaction cross section coverage, extending from 393 nuclides to 423 nuclides;
2. R-matrix analyses of neutron reactions on light nuclei, including isotopes of He, Li, and Be;
3. Resonance parameter analyses at lower energies and statistical high energy reactions for isotopes of Cl, K, Ti, V, Mn, Cr, Ni, Zr and W;
4. Modifications to thermal neutron reactions on fission products (isotopes of Mo, Tc, Rh, Ag, Cs, Nd, Sm, Eu) and neutron absorber materials (Cd, Gd);
5. Improved minor actinide evaluations for isotopes of U, Np, Pu, and Am (we are not making changes to the major actinides $^{235,238}\text{U}$ and ^{239}Pu at this point, except for delayed neutron data and covariances, and instead we intend to update them after a further period of research in experiment and theory), and our adoption of JENDL-4.0 evaluations for isotopes of Cm, Bk, Cf, Es, Fm, and some other minor actinides;
6. Fission energy release evaluations;
7. Fission product yield advances for fission-spectrum neutrons and 14 MeV neutrons incident on ^{239}Pu ; and

The ENDF/B-VII.1 library contains evaluations for 423 nuclides. The elemental evaluations for vanadium and zinc were replaced with isotopic evaluations and several other evaluations were added for a total of 32 new evaluations in ENDF/B-VII.1.

The evaluations that were added in ENDF/B-VII.1:

1. ^{50}V	12. ^{180}Ta	23. ^{240}Cm
2. ^{51}V	13. ^{180}W	24. ^{245}Bk
3. ^{64}Zn	14. ^{203}Tl	25. ^{246}Bk
4. ^{65}Zn	15. ^{205}Tl	26. ^{247}Bk
5. ^{66}Zn	16. ^{231}Th	27. ^{248}Bk
6. ^{67}Zn	17. ^{229}Pa	28. ^{246}Cf
7. ^{68}Zn	18. ^{230}Pa	29. ^{248}Cf
8. ^{70}Zn	19. ^{230}U	30. ^{251}Es
9. ^{168}Tm	20. ^{231}U	31. ^{252}Es
10. ^{169}Tm	21. ^{234}Np	32. $^{254m1}\text{Es}$
11. ^{170}Tm	22. ^{240}Am	

Or given in ZA space:

1. 23050	6. 30067	11. 69170
2. 23051	7. 30068	12. 73180
3. 30064	8. 30070	13. 74180
4. 30065	9. 69168	14. 81203
5. 30066	10. 69169	15. 81205

16. 90231	22. 95240	28. 98246
17. 91229	23. 96240	29. 98248
18. 91230	24. 97245	30. 99251
19. 92230	25. 97246	31. 99252
20. 92231	26. 97247	32. 99654
21. 93234	27. 97248	

1.4 Modifications to ENDF/B-VII.1 in ENDF71x

While the ACE data library is based upon ENDF/B-VII.1 the Nuclear Data Team has made a few modifications to the original ENDF/B-VII.1 data. These changes were made as problems were found and corrected. Only the problems where the ENDF/B file could be easily changed were fixed. They are documented below. The other problems require more substantial changes to the ENDF/B file. Those problems are documented in Section 2.

⁵⁶Fe In our visual inspection (see Section 3.3) we found that the elastic scattering ($|MT2$) cross sections went to 0.0 barn at an energy of 1.1971 MeV; when processed through NJOY, the resulting cross section value was 1×10^{-8} barn. The elastic scattering and other important cross sections are shown in Figure 1a; it is clear that the very low cross section value is too small. We modified the ENDF/B file to replace the 0.0 barn cross section with 1×10^{-6} barn. This value for the cross section was chosen as the smallest reasonable value.[10] The modified ENDF/B file was processed to create an ACE data table. The new cross section plot is shown in Figure 1b.

⁶¹Ni Similarly to ⁵⁶Fe, ⁶¹Ni had some unreasonable small elastic scattering ($MT=2$) cross section values. The original ACE data table cross sections are shown in Figure 2a. The energies at which the elastic scattering cross section is unreasonably small are 0.742 925 1 MeV to 0.743 962 MeV and 0.818 412 0 MeV which corresponds to four cross section values that are too small. The ENDF/B file was modified and reprocessed to create a new ACE data table. The modified cross sections are shown in Figure 2b. The cross sections are smaller than they were previously, but are still much smaller than the surrounding values. Additional work is required before the true value of the cross section is found.

2 Warnings and Issues

Using SZAX instead of ZAID with MCNP5 and MCNPX. MCNP5 and MCNPX do not—and will not—understand a SZAX. In all of the beta releases and at least the first production version of MCNP6 will also not be able to properly handle a SZAX. Future versions of MCNP6 will be able to understand and properly use a SZAX instead of a ZAID.

For those versions of MCNP that can't use a SZAX, problems can arise if a SZAX is specified instead of a ZAID. If a user enters 92235.710nc (hoping for ENDF/B-VII.1-based, room temperature ²³⁵U), the code will not crash, but will use 92235.71c (ENDF/B-VII.0-based, 600 K ²³⁵U) instead. The SZAX entries will be the last ones in the xsdir file and so are only found when the full SZAX is specified. Please make sure that what MCNP uses for its data is what you desired.

Negative PDF in ^{153}Eu Negative PDF values were found in MT=91 for ^{153}Eu . The negative values were set to zero and the distributions were renormed to integrate to 1 in the distributed ACE tables for ^{153}Eu . See Section 3.1 for more details.

Unresolved Resonances There appears to be problems with the unresolved resonances for the following evaluations:

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

These evaluations were processed with NJOY without the PURR module; the cross section values for the unresolved resonance range are taken directly from the MF=3 section of the ENDF/B file. See Section 3.1 for more information.

Negative Heating Values There were a combined 8624 negative heating values in 41 evaluations as found by `check_heat`. The problem evaluations are:

- | | | |
|----------------------|-------------------------|-----------------------|
| 1. ^{33}S | 15. $^{115m1}\text{Cd}$ | 29. ^{168}Tm |
| 2. ^{36}S | 16. ^{132}Te | 30. ^{174}Hf |
| 3. ^{59}Ni | 17. $^{129M1}\text{Te}$ | 31. ^{176}Hf |
| 4. ^{92}Zr | 18. ^{143}Ce | 32. ^{177}Hf |
| 5. ^{93}Zr | 19. ^{145}Nd | 33. ^{178}Hf |
| 6. ^{94}Zr | 20. ^{147}Nd | 34. ^{179}Hf |
| 7. ^{95}Zr | 21. ^{147}Sm | 35. ^{180}Hf |
| 8. ^{96}Zr | 22. ^{149}Sm | 36. ^{197}Au |
| 9. ^{93}Nb | 23. ^{151}Sm | 37. ^{196}Hg |
| 10. ^{92}Mo | 24. ^{153}Gd | 38. ^{202}Hg |
| 11. ^{94}Mo | 25. ^{155}Gd | 39. ^{203}Tl |
| 12. ^{96}Mo | 26. ^{165}Ho | 40. ^{205}Tl |
| 13. ^{97}Mo | 27. $^{115m1}\text{Ho}$ | 41. ^{209}Bi |
| 14. ^{98}Mo | 28. ^{166}Er | |

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.

Law 4 MCNP Bug ENDF/B-VII.1 contains some secondary gamma distributions that are formatted differently from what has been available in the past. The difference occurs when the ACE Law 4 is used to describe a discrete and continuum distributions for secondary gammas. In our testing we found that this data could cause older versions of MCNP (i.e., < MCNP6) to crash. This has been fixed in MCNP6. For more detailed information see Section 3.2.1.

All of the evaluations where this could be a problem occurs in data that was taken from the JENDL-4 library. The affected evaluations are:

- | | | |
|-----------------------|-----------------------|-----------------------|
| 1. ^{226}Ac | 11. ^{246}Pu | 21. ^{250}Cf |
| 2. ^{227}Th | 12. ^{243}Cm | 22. ^{251}Cf |
| 3. ^{228}Th | 13. ^{245}Cm | 23. ^{252}Cf |
| 4. ^{230}Th | 14. ^{247}Cm | 24. ^{253}Cf |
| 5. ^{233}Th | 15. ^{248}Cm | 25. ^{254}Cf |
| 6. ^{234}Th | 16. ^{249}Cm | 26. ^{252}Es |
| 7. ^{230}Pa | 17. ^{246}Bk | 27. ^{253}Es |
| 8. ^{232}U | 18. ^{248}Bk | 28. ^{255}Es |
| 9. ^{235}Np | 19. ^{249}Bk | |
| 10. ^{242}Pu | 20. ^{246}Cf | |

Too Many Secondaries in $^{231,233}\text{Pa}$ The number of secondary neutrons for MT=5 for $^{231,233}\text{Pa}$ is unphysically large for incident energies > 28 MeV. MCNP only tracks 11 secondary neutrons; if more than 11 neutrons are released in the reaction, problems occur that may cause MCNP to crash. This issue is discussed in more detail in Section 3.2.1. Care should be taken when using $^{231,233}\text{Pa}$ with incident neutron energies above 28 MeV.

Unphysically Large Elastic Scattering Cross Sections We feel that the elastic scattering (MT=2) cross sections in ^{237}U and ^{238}Pu are unphysically large. This is a deficiency in the ENDF/B evaluation file and not a result of our processing.

3 Testing

The entire ENDF71x release is 16 GiB in size.³ With such a large amount of data, it is impossible to check it manually. We have performed an extensive amount of testing on the ENDF/B-VII.1-based ACE data tables, more than any previous ACE data release from the Nuclear Data Team at LANL. This has been done in two separate, but concurrent, processes. The first is to verify that the data is correctly formatted with the second process to validate that the data interacts properly with MCNP. Both processes performed verification checks of the underlying physics. (We are concerned that we accurately represent the physics!)

Finally we have performed a visual inspection (see Section 3.3) of the room temperature cross sections for these reactions: 1) total, 2) absorption, 3) elastic scattering, 4) $(n, 2n)$, 5) fission, and 6) average heating number. The purpose of the visual inspection was to find gross errors in the cross section values.

Verification and validation is extremely important to the Nuclear Data Team. We recognize the trust that is placed on our data and know that once the data has been distributed there is no mechanism to recall the data if a problem is found. The verification process is described in Section 3.1 with the validation process described in Section 3.2.

³For comparison, the size of all the data in the previous release, i.e., ENDF/B-VII.0-based and older, historical data, was 12 GiB.

With that being said, we are somewhat at the mercy of the data evaluators, those who create the ENDF/B data files. If the ENDF/B data is wrong, or malformed, we are limited in the corrections we can provide. We can, however, raise a warning when issues arise; those warnings are given in Section 2. In general, the ENDF/B-VII.1 data release is of the highest quality that can be found and thus, there are few cases where the data is suspect.

3.1 Verification of Data with checkace

The Nuclear Data Team at LANL have developed a series of small programs used to verify the quality of ACE data tables. These small programs are driven by a script called `checkace`. This script and programs were run on all of the room temperature ACE data tables with the assumption being made that checking just the room temperature cases would find the problems in the remaining temperatures—there wouldn't be anything found in the higher temperature data tables that wouldn't be caught in the room temperature data. The only change in the processing between temperatures was the input of the desired temperature so additional problems should not be introduced simply by changing the temperature on the NJOY input card(s).

The checks that `checkace` and its subprograms perform are detailed in the paragraphs that follow. This same set of scripts and programs were used to test the ENDF/B-VII.0-based ACE data [5, Section 3.2.3] although we have made a few minor modifications to help us identify false positives.

You will note that all but one of the descriptions are the comments from the source code of the checking programs. The lone exception is that from `check_ures`.

check0

```
c   This code reads a Type-1 MCNP library and checks to make sure that
c   all threshold reactions have a leading zero in their cross-section
c   tabulation. It checks neutron cross sections, type-13 photon-
c   production cross sections, and other particle production cross
c   sections.
```

Nothing of significance was found by `check0`.

check5

```
c   This code reads in a type 1 MCNP data library and checks
c   the information for MT=5. The code prints out the
c   threshold energy and the first (energy, yield) pair for secondary
c   neutrons. It is checking to see if the threshold for MT=5
c   is lower than the first data pair, then the first yield MUST BE
c   zero. If it finds that the first energy is less than the
c   threshold and that the yield is non 0.0, then it prints a message.
```

Nothing of significance was found by `check5`.

check61

```
c   The program check61 reads in an MCNP type 1 library file
c   and checks various aspects of the secondary neutron energy
c   distributions which use LAW=61. It verifies that
c   interpolation schemes 1 or 2 are used, and identifies any
c   negative probability density functions. The code checks to
c   see if any secondary neutrons are produced with energy greater
c   than the incident neutron energy and takes corrective action.
c   Of course fission is not corrected. It will also fix the
c   negative probabilities by setting them to zero.
```

With check61 a negative PDF was found for MT=91 in the ^{153}Eu evaluation. Negative PDFs are truly unphysical. The negative PDF was found in the original ENDF/B file and so is not a consequence of NJOY processing.

When check61 finds a negative PDF, it replaces the negative values with zeros, renorms the distribution, and writes a new ACE file. This modified ACE file was used instead of the file that comes out of NJOY.

check_heat

```
c   This code reads in a type 1 MCNP data library and checks
c   various aspects of heating numbers. first it checks the main
c   heating grid for zeros or negatives. If there are negative
c   heating numbers then it prints an error; if there are zeros then
c   it prints a warning (which can probably be ignored).
c
c   Then it checks each of the partial particle heating arrays for
c   the same features. finally, it totals these partial heating
c   arrays and does some comparisons of this total to the main grid.
```

There were a combined 8624 negative heating values in 41 evaluations as found by check_heat. The problem evaluations are:

- | | | |
|----------------------|-------------------------|-----------------------|
| 1. ^{33}S | 12. ^{96}Mo | 23. ^{151}Sm |
| 2. ^{36}S | 13. ^{97}Mo | 24. ^{153}Gd |
| 3. ^{59}Ni | 14. ^{98}Mo | 25. ^{155}Gd |
| 4. ^{92}Zr | 15. $^{115m1}\text{Cd}$ | 26. ^{165}Ho |
| 5. ^{93}Zr | 16. ^{132}Te | 27. ^{566}Ho |
| 6. ^{94}Zr | 17. ^{529}Te | 28. ^{166}Er |
| 7. ^{95}Zr | 18. ^{143}Ce | 29. ^{168}Tm |
| 8. ^{96}Zr | 19. ^{145}Nd | 30. ^{174}Hf |
| 9. ^{93}Nb | 20. ^{147}Nd | 31. ^{176}Hf |
| 10. ^{92}Mo | 21. ^{147}Sm | 32. ^{177}Hf |
| 11. ^{94}Mo | 22. ^{149}Sm | 33. ^{178}Hf |

- | | | |
|-----------------------|-----------------------|-----------------------|
| 34. ^{179}Hf | 37. ^{196}Hg | 40. ^{205}Tl |
| 35. ^{180}Hf | 38. ^{202}Hg | 41. ^{209}Bi |
| 36. ^{197}Au | 39. ^{203}Tl | |

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.

When negative (or zero) values of the heating value are plotted on log-log plot (as is typically done for cross sections), a gap is seen in the plot. An example of a gap in the average heating values can be seen in Figure 3 where a large gap in the average heating value can be seen around 1 MeV.

Independently, MacFarlane [11, 12], found a number of problems with kerma values, average heating, and missing photon energy production. Every evaluation that was flagged problematic by `check_heat` was also found to be problematic by MacFarlane as well. These are problems with the original ENDF/B file and corrections need to be made there. Please see MacFarlane's work at <http://t2.lanl.gov/data/endl/ebalVII/summary.html>.

check_ures *This program analyzes the unresolved resonance probability tables generated by the PURR module of NJOY to assure that the partial cross sections or factors add up appropriately to totals and that no unrealistic heating values exist. It lists all the cross sections and factors for each incident energy and prints warning messages when partials do not add up correctly to the total within 1 and/or 5%, if some values are zero, or if unrealistic heating numbers exist. All errors given in the output file are transmitted to the log file by CHECKACE.PL as are the total number of potential problems identified by check_ures.*

There were 15 evaluations that had significant problems with their unresolved resonance probability tables. These evaluations were reprocessed by NJOY without using the PURR module; the cross section values for the unresolved resonance range in the ACE data table are the average cross section values given in MF=3 of the ENDF/B file. The evaluations that we processed without using the PURR module are:

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

ENDF/B-VII.0 also had a number of evaluations with unresolved resonance parameters as documented by Trellue, Little, and Lee [5]. The Nuclear Data Team feel that the unresolved resonance range for these evaluations need to be examined and updated in their ENDF file.

checknd

```

c   The program checknd reads in an MCNP type 1 library file
c   and checks various aspects of the secondary photon energy
c   distributions which use LAW=4 or 44. It informs the user
c   if the secondary photon energies are discrete and if there are

```

```
c    any negative discrete energies at adjacent incident neutron
c    energies.
```

Nothing of significance was found by checknd.

checknd_neut

```
c    The program checknd_neut reads in an MCNP type 1 library file
c    and checks various aspects of the secondary neutron energy
c    distributions which use LAW=4 or 44. It verifies that
c    interpolation schemes 1 or 2 are used, and identifies any negative
c    probability density functions. The code checks to see if any
c    secondary neutrons are produced with energy greater than the
c    incident neutron energy and takes corrective action. Of course
c    fission is not corrected. It will also fix the negative probabilities
c    by setting them to zero.
```

Nothing of significance was found by checknd_neut.

checkthresh

```
c    This code reads in a type 1 MCNP data library and
c    checks the reaction threshold energies with the
c    kinematic thresholds for negative Q-value reactions.
c    If the library threshold is lower than the kinematic threshold
c    the codes outputs this information along with the magnitude
c    of the discrepancy, the law specified for the secondary neutrons
c    and the line number on the type 1 library file containing the
c    problem energy value. If no error are detected no print out is
c    given.
```

Nothing of significance was found by checkthresh.

checkxs

```
c    This program reads in a Type 1 MCNP library, and for each
c    zaid it compares the total cross section to the sum of the
c    partials for neutrons and for photon production. The user
c    is queried for all relevant information interactively.
```

Nothing of significance was found by checkxs.

3.2 Validation through Mechanical Testing With MCNP6 and MCNP5

A number of “mechanical” tests have been performed to ensure—at the very least—that the ACE data tables don’t cause MCNP to crash. These tests consisted of four fixed-source calculations that were performed for every combination of nuclide and temperature available in ENDF71x using both MCNP6 and MCNP5. With the exception of material- and temperature-dependent parameters (e.g., density, which was chosen to be the maximum of nominal density and unit density [1 g cm^{-3}] for each nuclide), the input files for a given fixed-source calculation were identical. A sample MCNP input deck that we used is shown in Appendix B.

Three fixed-source calculations were performed using an isotropic point neutron source at the origin surrounded by a uniform sphere (4 cm radius) composed of a single nuclide. The energy spectrum of the point neutron source was given by 1) a log-uniform distribution on the entire interval covered by the main energy grid of the appropriate ACE file, 2) a Watt fission spectrum, or 3) a room-temperature Maxwell-Boltzmann distribution. A fourth fixed-source calculation used the same log-uniform distribution of neutron energies as the first, but the source was uniformly distributed throughout the volume of the sphere. Neutrons and secondary photons (i.e., mode `n p`) were transported in these calculations.

Tallies of the current across the outer surface of the sphere (F1), the flux at the outer surface of the sphere (F2), and the average flux within the sphere (F4) were performed for both neutrons and photons. Each tally was defined to have 500 logarithmically-spaced energy bins. The neutron tallies covered the entire energy range for which cross section data exists for a given isotope in ENDF71x, while for photon tallies the lower end of this energy range was truncated at 1 keV, the minimum cutoff energy for photons in MCNP. One billion source neutrons were tracked in each calculation, and no computer time limit was imposed. After all of these test calculations were completed, the output files generated by MCNP were checked for major errors.

3.2.1 Crashes of MCNP Encountered During Mechanical Testing

During our mechanical testing of the ENDF71x data tables, we discovered two problems that caused MCNP6 to crash. Our investigation of these problems revealed that they are symptomatic of issues that affect MCNP5, MCNPX and earlier versions of MCNP.

Law 4 Bug The first crash occurred during a test calculation that used the volumetric neutron source, a sphere of ^{226}Ac , and a temperature of 1200 K. During the problematic history, a secondary photon was generated from an $(n, 4n)$ reaction with a clearly unphysical energy of -3.5767 GeV . When MCNP6 encountered this negative photon energy, it issued an error message and aborted execution.

We have determined that this crash occurred because of a bug in the MCNP code. In ENDF71x, secondary photon energy distribution data for the ^{226}Ac $(n, 4n)$ reaction are given using ENDF Law 4. Law 4 represents the distribution of secondary photon energies for a reaction using a table of incident neutron energies. For each incident neutron energy given on the table, the secondary photon energy distribution may be represented using discrete lines, a continuum, or both. While MCNP requires that each incident neutron energy should use the same number of discrete lines, there is no similar requirement for the continua.

Before this crash was fully investigated, MCNP6 assumed during interpolation between two incident neutron energies on a Law 4 table that neighboring entries would always either both contain or neither contain a continuum distribution. When this assumption was violated during our test calculation, MCNP “jumped off” the edge of the table and used unrelated data to sample the energy of a secondary photon. MCNP6 caught the error and crashed in this instance because the photon energy happened to be negative. However, positive energies that are incorrectly sampled because of this bug will be accepted quietly by the code.

The MCNP Development Team has now corrected this issue in MCNP6 and has published a technical report describing the bug fix [13]. Our investigation revealed that this error may still occur (although rarely) for photons sampled from (n, xn) reactions when ENDF71x data for the following minor actinides are used with versions of MCNP older than MCNP6.

- | | | |
|-----------------------|-----------------------|-----------------------|
| 1. ^{226}Ac | 11. ^{246}Pu | 21. ^{250}Cf |
| 2. ^{227}Th | 12. ^{243}Cm | 22. ^{251}Cf |
| 3. ^{228}Th | 13. ^{245}Cm | 23. ^{252}Cf |
| 4. ^{230}Th | 14. ^{247}Cm | 24. ^{253}Cf |
| 5. ^{233}Th | 15. ^{248}Cm | 25. ^{254}Cf |
| 6. ^{234}Th | 16. ^{249}Cm | 26. ^{252}Es |
| 7. ^{230}Pa | 17. ^{246}Bk | 27. ^{253}Es |
| 8. ^{232}U | 18. ^{248}Bk | 28. ^{255}Es |
| 9. ^{235}Np | 19. ^{249}Bk | |
| 10. ^{242}Pu | 20. ^{246}Cf | |

For all of these nuclides, the problematic Law 4 data were added in the ENDF/B-VII.1 release and were borrowed from JENDL-4.0 [14].

Many Secondaries Bug The second problem that caused MCNP to crash occurred because of incorrect secondary neutron yields that are tabulated for $^{231,233}\text{Pa}$ in ENDF/B-VII.1. For the MT=5 reaction,⁴ unrealistically large neutron yields (see Figure 4) are given in the high-energy range (about >20 MeV) for both of these isotopes. These unphysical neutron yields were added in ENDF/B-VII.0 and remain unchanged in ENDF/B-VII.1.

All currently extant versions of MCNP assume that the number of secondary neutrons produced by a single instance of certain reactions will never exceed 11. When one of the reactions for which this assumption is made produces more than 11 secondary neutrons, MCNP modifies data stored in memory near the array describing the secondary neutrons. The result of these haphazard modifications to unrelated data depends on how memory is allocated at run-time, but our test calculations suggest that crashes due to segmentation faults are typical. This problem is currently under investigation by the MCNP Development Team.

⁴MT=5 is a catch-all reaction that represents everything not already accounted for in the other reactions.

3.3 Visual Inspection of Major Cross Sections

The previous sections have shown how we have attempted to find problems with the data using checking codes and running simulations. However, there are some things that can only be found by the human eye.

We have plotted these reactions: 1) total, 2) absorption, 3) elastic scattering, 4) $(n, 2n)$, and 5) average heating number (kerma times total cross section). These data were chosen to be plotted because they are important reactions or because we have had complications with them in the past. The data was taken from our ACE data tables, but originates in the ENDF/B files.

The cross sections were plotted *for every evaluation* and we have visually inspected every plot looking for errors in the data. This inspection was intended to catch gross errors and not the minute problems that might occur. In the paragraphs that follow is described the issues that we have found.

Sawtooth Cross Sections We found a number of evaluations with unphysical changes in the cross section value of several orders of magnitude. These large unphysical changes appear to have a “sawtooth” in the plot of the cross section. The large change in the cross section is not limited to the ACE data tables, but is an issue with the ENDF/B files themselves.

A typical example of the sawtooth-like pattern is shown in Figure 5 where we can see a large drop in the cross sections at a little less than an eV. The list of evaluations that have this pattern is given below.

1. ^{58m1}Co	22. ^{131}I	43. ^{229}Pa
2. ^{65}Zn	23. ^{124}Xe	44. ^{230}U
3. ^{79}Se	24. ^{133}Xe	45. ^{231}U
4. ^{78}Kr	25. ^{134}Xe	46. ^{241}U
5. ^{89}Sr	26. ^{136}Cs	47. ^{235}Np
6. ^{90}Sr	27. ^{137}Cs	48. ^{239}Np
7. ^{91}Y	28. ^{144}Ce	49. ^{246}Pu
8. ^{95}Nb	29. ^{148}Pm	50. ^{243}Am
9. ^{99}Mo	30. ^{149}Pm	51. ^{240}Cm
10. ^{96}Ru	31. ^{156}Eu	52. ^{241}Cm
11. ^{98}Ru	32. ^{223}Ra	53. ^{249}Cm
12. ^{105}Ru	33. ^{224}Ra	54. ^{245}Bk
13. ^{106}Ru	34. ^{225}Ra	55. ^{247}Bk
14. ^{105}Rh	35. ^{225}Ac	56. ^{248}Cf
15. ^{123}Sn	36. ^{226}Ac	57. ^{251}Cf
16. ^{126}Sn	37. ^{227}Ac	58. ^{253}Cf
17. ^{124}Sb	38. ^{227}Th	59. ^{254}Cf
18. ^{125}Sb	39. ^{228}Th	60. ^{251}Es
19. ^{120}Te	40. ^{231}Th	61. ^{254}Es
20. $^{129m1}\text{Te}$	41. ^{233}Th	62. ^{255}Es
21. $^{127m1}\text{Te}$	42. ^{234}Th	

Average Heating Gaps Another problem discovered in the visual inspection of the cross sections is gaps in the average heating value. A gap in the plot of the average heating value occurs when the average heating value is zero or negative.

A typical example of the gap in the average heating values was shown previously in Figure 3 where a large gap in the average heating value is seen around 1 MeV. The list of evaluations that have this pattern is given below. The heating problems shown in these evaluations have been confirmed by Bob MacFarlane [12, 11]

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

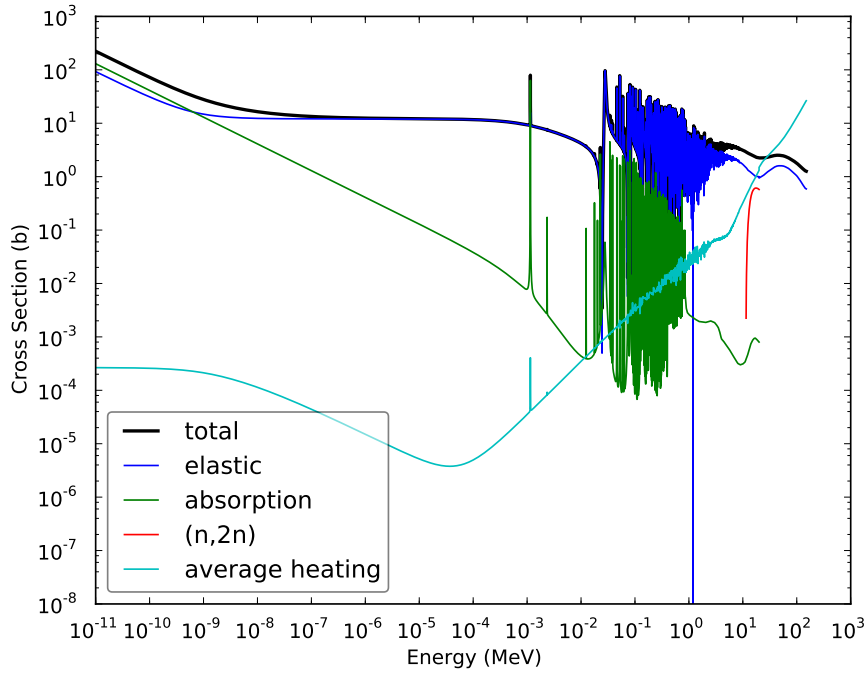
Unphysically Small Elastic Scattering Cross Sections Two evaluations— ^{56}Fe and ^{61}Ni —had elastic scattering (MT=2) cross sections that were much too small. Upon closer inspection of the ENDF/B file, we discovered that the cross sections went to 0.0 which we don't believe is accurate. The ENDF/B files for these two isotopes were modified as explained in Section 1.4.

Unphysically Large Elastic Scattering Cross Sections In contrast to the small elastic scattering cross sections in ^{56}Fe and ^{61}Ni , we feel that the elastic scattering (MT=2) cross sections in ^{237}U and ^{238}Pu are unphysically large. This is a deficiency in the ENDF/B evaluation file and not a result of our processing.

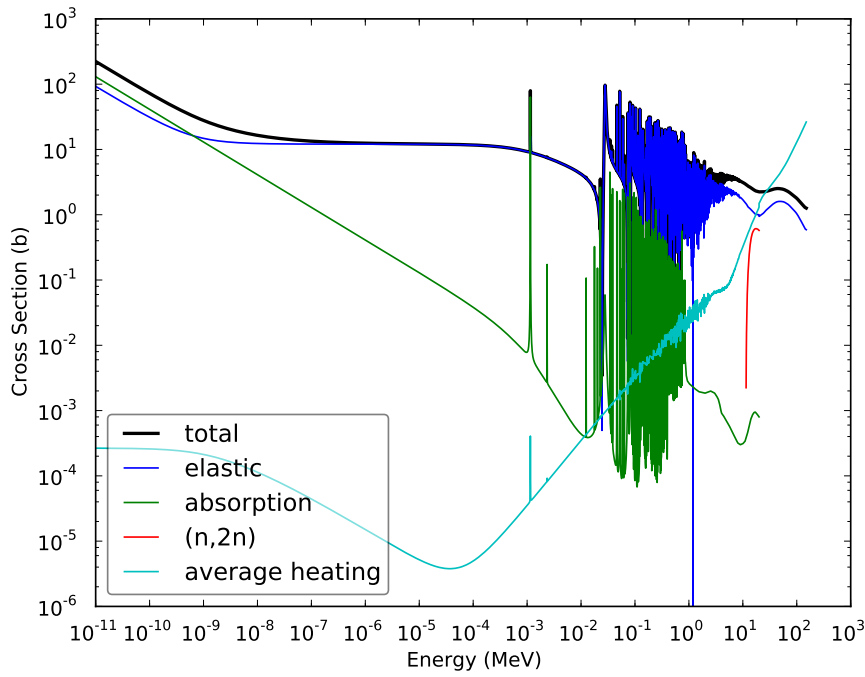
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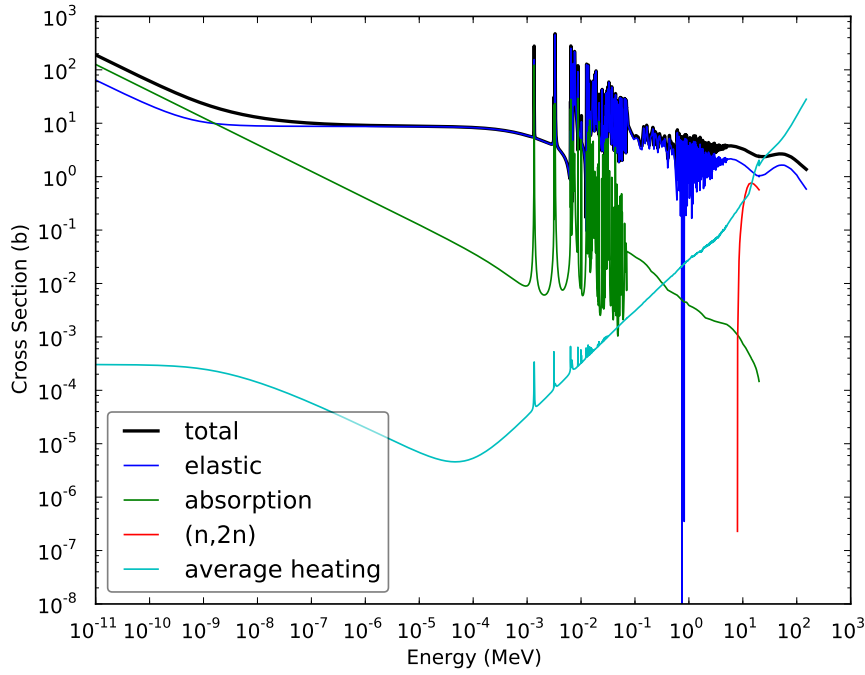


(a) Unmodified

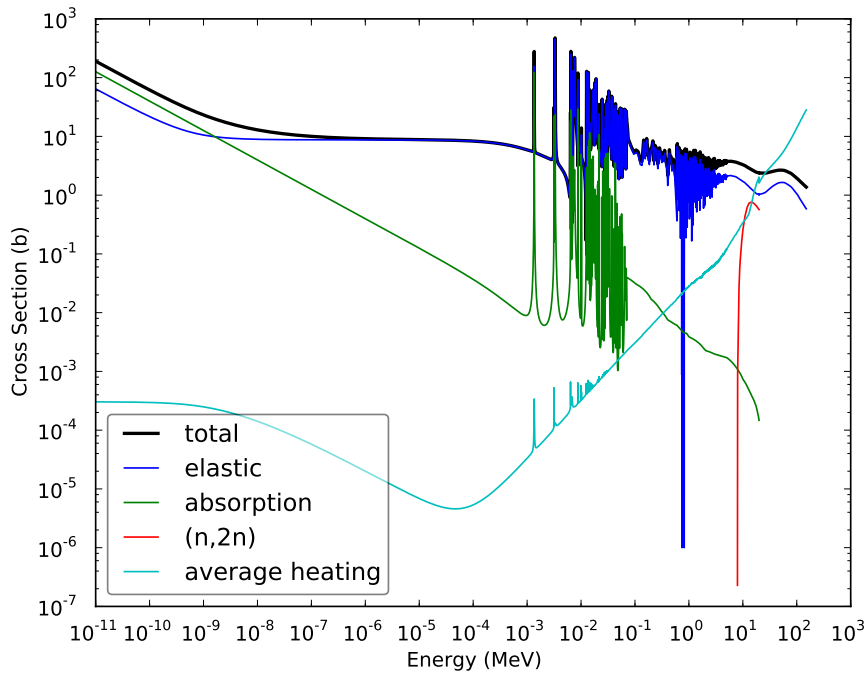


(b) Modified

Figure 1: Cross section plot of the total, elastic, absorption, and $(n, 2n)$ cross sections of ^{56}Fe as well as the average heating. Note the difference in scales of the ordinates.



(a) Unmodified



(b) Modified

Figure 2: Cross section plot of the total, elastic, absorption, and $(n, 2n)$ cross sections of ^{61}Ni as well as the average heating.

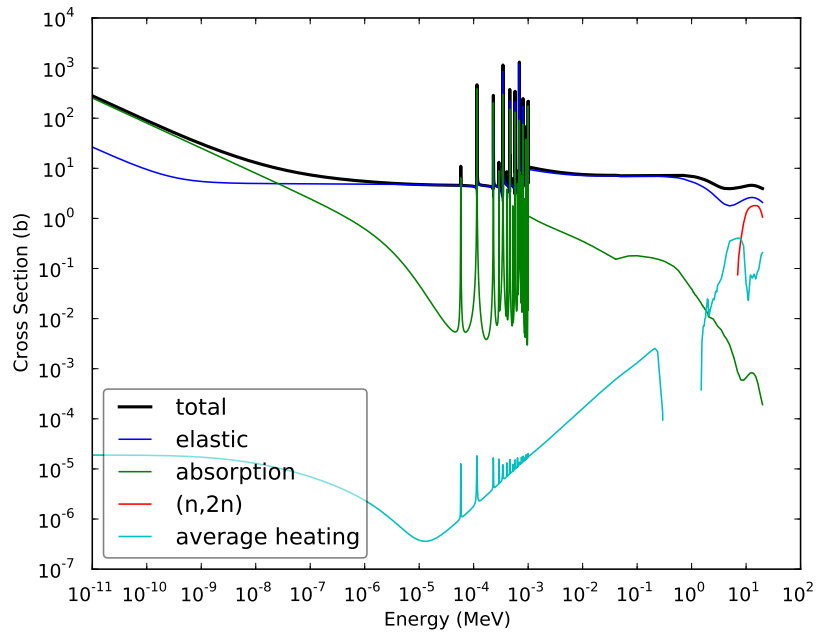


Figure 3: Plot of the “major” $^{115m1}\text{Cd}$ cross sections showing the unphysical gaps in the average heating value around 1 MeV.

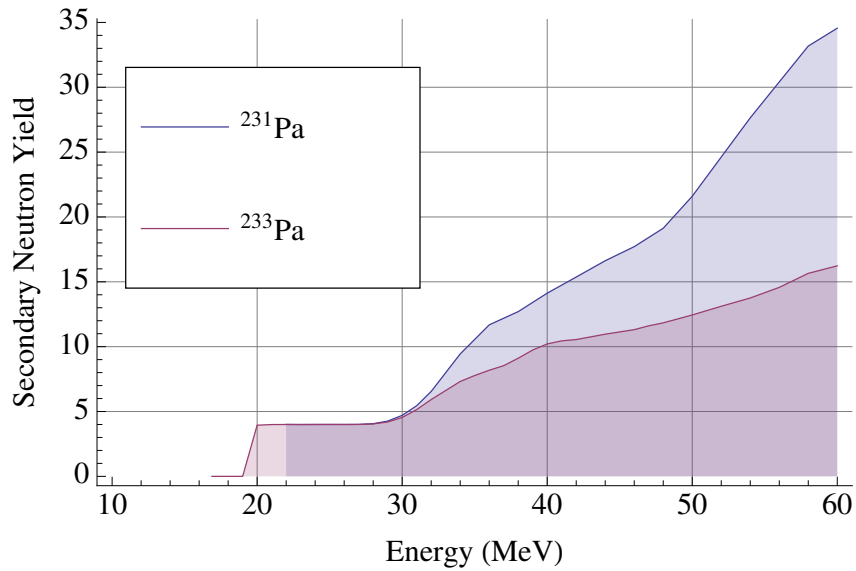


Figure 4: Plot of the ^{231}Pa (blue) and ^{233}Pa (purple) secondary neutron yields for MT=5 showing the unphysical values above about 30 MeV.

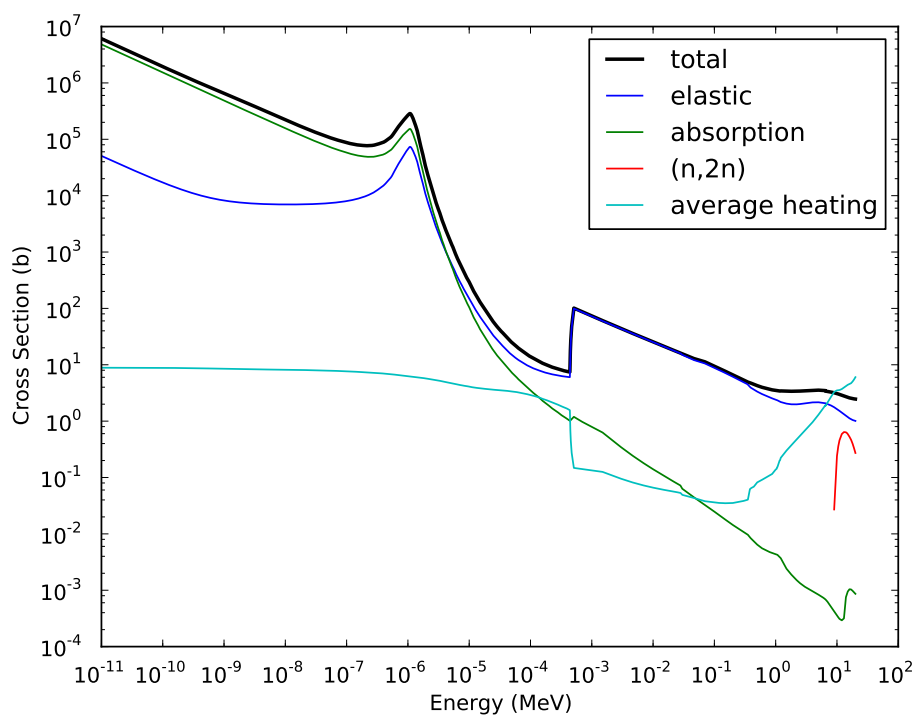


Figure 5: Plot of the “major” ^{58m1}Co cross sections showing the unphysical, sawtooth-like problem.

A Typical NJOY Input Deck

Listed below is a typical NJOY input deck used in the processing of the ENDF/B-VII.1 files into an ACE data table.

```
moder
 20 -30 /
reconr
-30 -31 /
'automated processing using ndvv.njoy.process see *.log files' /
9228 0 0 /
0.001 0.0 0.01 5.0000000000000004e-08 /
0 /
moder
-31 21 /
moder
 21 -31 /
broadr
-30 -31 -32 /
9228 1 0 0 0.0 /
0.001 1000000.0 0.01 5.0000000000000004e-08 /
293.6
0 /
heatr
-30 -32 -33 /
9228 3 0 0 0 2 /
442
443
444
gaspr
-30 -33 -34 /
moder
-34 -35 /
moder
-35 22 /
purr
 20 21 22 /
9228 1 1 16 64 1 /
293.6 /
10000000000.0 /
0 /
acer
 20 22 0 23 24 /
 1 0 1 0.000000 /
'U235 ENDF71x (jlconlin) Ref. see jlconlin (ref 09/10/2012 10:00:53)' /
9228 293.6 /
 1 1 /
 /
acer
 0 23 0 25 26 /
 7 1 1 0.800000 /
'U235 ENDF71x (jlconlin) Ref. see jlconlin (ref 09/10/2012 10:00:53)' /
stop
```

B MCNP Input File For Testing

Shown here is a sample MCNP input file that we used for our testing. The source definition would be changed in this for the different energy sources we have tested.

```
Iron-56 Sphere at the Origin
C
C *** Block 1: Cells ***
1 1 -7.874 -1 imp:n,p=1 $ Sphere of iron-56 centered at the origin
2 0 1 imp:n,p=0 $ The world outside of the sphere doesn't matter

C *** Block 2: Surfaces ***
1 so 4 $ Sphere centered at the origin (4 cm radius)

C *** Block 3: Data ***
MODE n p $ Track neutrons and photons
M1 26056.80c 1.0000 $ Iron-56 at room temperature
C
TMP 2.530100E-08 2.530100E-08 $ The entire universe is at room temperature
C
C The source emits neutrons with energies given by a log-uniform distribution
C over the interval [1e-11 MeV, 150 MeV] This distribution is approximated by a
C histogram with 1500 equally-probable logarithmically-spaced bins.
SDEF pos=0 0 0 erg=d1 $ Isotropic point source at the origin.
SI1 H 1.000e-11 1498ilog 1.500e2
C All the bins are equally probable. Note that MCNP is smart enough to
C normalize this properly, so we can just use 1 as the probability for each bin.
SP1 D 0 1 1498r
C
F1:N 1 $ Surface current tally for neutrons leaving the sphere.
E1 1.000e-11 498ilog 1.500e2 $ 500 logarithmically-spaced energy bins
FC1 Surface current of neutrons leaving the Iron-56 sphere
F11:P 1 $ Surface current tally for photons leaving the sphere.
E11 1.000e-3 498ilog 1.500e2 $ 500 logarithmically-spaced energy bins
FC11 Surface current of photons leaving the Iron-56 sphere
F2:N 1 $ Surface flux tally for neutrons leaving the sphere.
E2 1.000e-11 498ilog 1.500e2 $ 500 logarithmically-spaced energy bins
FC2 Surface flux of neutrons leaving the Iron-56 sphere
F12:P 1 $ Surface flux tally for photons leaving the sphere.
E12 1.000e-3 498ilog 1.500e2 $ 500 logarithmically-spaced energy bins
FC12 Surface flux of photons leaving the Iron-56 sphere
F4:N 1 $ Volume flux tally for neutrons inside the sphere.
E4 1.000e-11 498ilog 1.500e2 $ 500 logarithmically-spaced energy bins
FC4 Average flux of neutrons within the Iron-56 sphere
F14:P 1 $ Volume flux tally for photons inside the sphere.
E14 1.000e-3 498ilog 1.500e2 $ 500 logarithmically-spaced energy bins
FC14 Average flux of photons within the Iron-56 sphere
C
C Use a maximum energy (Emax) equal to 5x the maximum energy on the ACE file
C energy grid for this isotope. Also turn all physics models off (only ACE data
C will be used).
PHYS:N 7.500e2 6j 1.500e3
C
C Perform a dump to the output file, the runtpe file, and the mctal file after
C every 1.000e9 histories and use the default mctal format. Also have the
C multiple processors rendezvous and write to the tally fluctuation chart every
C 1.000e8 particles.
PRDMP 1.000e9 1.000e9 1 J 1.000e8
C
NPS 1.000e9 $ Maximum number of particle histories
C
PRINT $ Print a full output file
```