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Title: Release of NDI Libraries MENDF80 and MT80—Libraries Based on ENDF/B-VIII.0

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memorandum

Materials & Physical Data (XCP-5)

SUBJECT: Release of NDI Libraries MENDF80 and MT80—Libraries Based on ENDF/B-VIII.0

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I. Introduction

Several new NDI libraries have been released by the Nuclear Data Team. There are multigroup-energy neutron libraries (see Section II.) and associated production-depletion libraries (see Section IV.). The libraries are based on data from ENDF/B-VIII.0[1]. The libraries will be available with NDI version 2.1.4 when it becomes available in Spring of 2020. These libraries are the libraries recommended for use by the Nuclear Data Team. We encourage all to adopt these libraries at their earliest convenience.

II. Multigroup-Energy Neutron Libraries

There are two multigroup-energy neutron libraries:

mendf80 room temperature only, down-scatter only, based on ENDF/B-VIII.0; and

mt80 multi-temperature, with up-scatter, based on ENDF/B-VIII.0.

These libraries use the 618_lanl group structure[2], which is the standard group structure at LANL for more than a decade. This is collapse-compatible with the oft-used 250_lanl 133_lanl, 70_lanl, and 30_lanl group structures. The SZAID IDs and associated temperatures are given in Table 1. Note that the mendf80 library is only at room-temperature (293.6 K) while the mt80 is available at 23 temperatures, the same temperature set[3] that we have used for the mt71x[4] library.

II.A. SZAs for Libraries

Tables 2–4 give a list of SZAs for both mendf80 and mt80. There are 557 evaluations from ENDF/B-VIII.0 and two fission products, 45117 for uranium fission products and 46119 for plutonium fission products[5]. In addition, we have created data for 25 elements by combining the data from all of the isotopic data for that element. Table 5 gives a list of SZAs for the elemental data in both mendf80 and mt80. For more information on the elemental data, please see Appendix A.

II.B. 30-Group, Pre-Collapsed, Libraries

In the past, we have delivered a pre-collapsed, 30-group version of some of our libraries to select customers. Due to popular demand, we are making available a 30-group version of mendf80 and mt80 for all of our customers. These pre-collapsed libraries have been collapsed directly from the 618-group libraries using NDI and use the 30_lanl group structure. The names of the 30-group libraries are mendf80_30g and mt80_30g

Table 1: SZAIDs and associated temperatures for data in the mendf80 and mt80 multigroup-energy neutron libraries

Library	SZAID ID	Temperature (K)
mendf80	800nc	293.6
	801nc	293.6
	802nc	1160.451
	803nc	2506.573
	804nc	11 604.505
	805nc	20 636.291
	806nc	35 973.966
	807nc	65 256.773
	808nc	116 045.05
	809nc	206 362.91
mt80	810nc	359 739.66
	811nc	652 567.73
	812nc	1 160 450.5
	813nc	2 063 629.1
	814nc	3 597 396.6
	815nc	6 525 677.3
	816nc	11 604 505.0
	817nc	20 636 291.0
	818nc	35 973 966.0
	819nc	65 256 773.0
	820nc	116 045 050.0
	821nc	359 739 660.0
	822nc	1 160 450 500.0
	823nc	3 597 396 600.0

Table 2: List of SZAs for light-weight (i.e., $Z < 25$) in the mendf80 and mt80 libraries.

	1001	1002	1003	2003	2004	3006	3007
4007	4009	5010	5011	6012	6013	7014	7015
8016	8017	8018	9019	10020	10021	10022	11022
11023	12024	12025	12026	1013026	13027	14028	14029
14030	14031	14032	15031	16032	16033	16034	16035
16036	17035	17036	17037	18036	18037	18038	18039
18040	18041	19039	19040	19041	20040	20041	20042
20043	20044	20045	20046	20047	20048	21045	22046
22047	22048	22049	22050	23049	23050	23051	24050
24051	24052	24053	24054	25054	25055		

Table 3: List of SZAs for mid-weight isotopes (i.e., $25 < Z \leq 88$) in the `mendf80` and `mt80` libraries. SZAs marked with a dagger (†) indicate fission product evaluations.

26054	26055	26056	26057	26058	27058	1027058	27059	28058
28059	28060	28061	28062	28063	28064	29063	29064	29065
30064	30065	30066	30067	30068	30069	30070	31069	31070
31071	32070	32071	32072	32073	32074	32075	32076	33073
33074	33075	34074	34075	34076	34077	34078	34079	34080
34081	34082	35079	35080	35081	36078	36079	36080	36081
36082	36083	36084	36085	36086	37085	37086	37087	38084
38085	38086	38087	38088	38089	38090	39089	39090	39091
40090	40091	40092	40093	40094	40095	40096	41093	41094
41095	42092	42093	42094	42095	42096	42097	42098	42099
42100	43098	43099	44096	44097	44098	44099	44100	44101
44102	44103	44104	44105	44106	45103	45104	45105	45117†
46102	46103	46104	46105	46106	46107	46108	46109	46110
46119†	47107	47108	47109	1047110	47111	47112	47113	47114
47115	47116	47117	1047118	48106	48107	48108	48109	48110
48111	48112	48113	48114	1048115	48116	49113	49114	49115
50112	50113	50114	50115	50116	50117	50118	50119	50120
1050121	50122	50123	50124	50125	50126	51121	51122	51123
51124	51125	51126	52120	52121	1052121	52122	52123	52124
52125	52126	1052127	52128	1052129	52130	52131	1052131	52132
1053132	53127	53128	53129	53130	53131	53132	53133	53134
53135	54123	54124	54125	54126	54127	54128	54129	54130
54131	54132	54133	54134	54135	54136	55133	55134	55135
55136	55137	56130	56131	56132	56133	56134	56135	56136
56137	56138	56139	56140	57138	57139	57140	58136	58137
1058137	58138	58139	58140	58141	58142	58143	58144	59141
59142	59143	60142	60143	60144	60145	60146	60147	60148
60149	60150	61143	61144	61145	61146	61147	61148	1061148
61149	61150	61151	62144	62145	62146	62147	62148	62149
62150	62151	62152	62153	62154	63151	63152	63153	63154
63155	63156	63157	64152	64153	64154	64155	64156	64157
64158	64159	64160	65158	65159	65160	65161	66154	66155
66156	66157	66158	66159	66160	66161	66162	66163	66164
67165	1067166	68162	68163	68164	68165	68166	68167	68168
68169	68170	69168	69169	69170	69171	70168	70169	70170
70171	70172	70173	70174	70175	70176	71175	71176	72174
72175	72176	72177	72178	72179	72180	72181	72182	73180
73181	73182	74180	74181	74182	74183	74184	74185	74186
75185	1075186	75187	76184	76185	76186	76187	76188	76189
76190	76191	76192	77191	77192	77193	1077194	78190	78191
78192	78193	78194	78195	78196	78197	78198	79197	80196
80197	1080197	80198	80199	80200	80201	80202	80203	80204
81203	81204	81205	82204	82205	82206	82207	82208	83209
1083210	84208	84209	84210	88223	88224	88225	88226	

Table 4: List of SZAs for actinides (i.e., $Z > 88$) in the mendlf80 and mt80 libraries.

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	1093236
93237	93238	93239	94236	94237	94238	94239	94240
94241	94242	94243	94244	94245	94246	95240	95241
95242	1095242	95243	95244	1095244	96240	96241	96242
96243	96244	96245	96246	96247	96248	96249	96250
97245	97246	97247	97248	97249	97250	98246	98247
98248	98249	98250	98251	98252	98253	98254	99251
99252	99253	99254	1099254	99255	100255		

Table 5: List of SZAs for elementals added to the mendlf80 and mt80 libraries.

6000	12000	14000	17000	18000	19000
20000	22000	23000	24000	26000	28000
29000	31000	40000	42000	47000	48000
49000	54000	63000	64000	72000	74000
77000	82000				

III. Issues

We encountered a few issues that required some manual manipulation of the data after the processing was complete.

III.A. Xenon-135

There was an issue processing ^{135}Xe at the highest temperature. We have simply copied the 54135.822nm file to 54135.823nm file and modified the SZAID by hand. The data for the two files are identical. Please note that the SZAID extensions 822nm and 823nm refers to the 22nd and 23rd temperature; 1 160 450 500.0 K and 3 597 396 600.0 K respectively.

III.B. Missing Fission- Q Data

There are a handful of materials that did not have fission Q data, thus there was no `fiss_q` array in the NDI data. To solve this, we have copied the `fiss_q` data from a “neighboring” isotope. Here are the materials with missing fission Q data and from where we got the `fiss_q` array data.

^{223}Ra Data taken from ^{223}Ra in the MENDF70x library[6].

^{226}Ra Data taken from ^{226}Ra in the MENDF70x library[6].

^{245}Pu Data taken from ^{243}Pu in the MENDF80 library.

^{247}Cf Data taken from ^{249}Cf in the MENDF80 library.

^{251}Es Data taken from ^{254}Es in the MENDF80 library.

^{252}Es Data taken from ^{254}Es in the MENDF80 library.

^{253}Es Data taken from ^{254}Es in the MENDF80 library.

$^{254m1}\text{Es}$ Data taken from ^{254}Es in the MENDF80 library.

^{255}Es Data taken from ^{254}Es in the MENDF80 library.

IV. Production-Depletion Libraries

There are three production-depletion libraries associated with the multigroup-energy neutron libraries:

- nosub.800** production-depletion chain that provides the reaction products for each target in the chain;
- full.800** production-depletion chain with substitution for reaction products for which multigroup-energy transport data are not available; and
- basic.800** production-depletion chain identical to **full.800** except for targets with $6 < Z < 80$ where the only product for each reaction is the target itself [7, 8].

All of the production-depletion chains are appropriate for use with either the **mendf80** or **mt80** libraries, depending on the fidelity of the production or depletion needed for your calculation. The production-depletion chains were calculated with a series of scripts[9]. The scripts also have the ability to check and the produced chains for validity. The chains were verified using the checking script and found to be correct.

These scripts have been updated to be more flexible for more libraries. The updated scripts can be found at <https://xcp-stash.lanl.gov/projects/NDT/repos/productioncompletioncreator>

V. Verification and Validation

We have performed some verification and validation tests on this data. The first step is always to run a suite of checks called **checkmg** [10]. These were run to look for simple, but critical, problems. The results of these checks did not uncover any major issues.

In addition to running **checkmg** several simulations have been performed and compared with previous nuclear data libraries. These simulations are documented in separate memos by Saller [11] and [12].

VI. Conclusion

The Nuclear Data Team has produced two new multigroup-energy neutron libraries; **mendf80**, a room-temperature only library with no up-scatter, and **mt80**, a multi-temperature library with up-scatter. Both libraries are based on ENDF/B-VIII.0. Three new production-depletion libraries have also been made to complement the multigroup-energy neutron libraries; **nosub**, **full**, and **basic**.

The generation of this library was several years in the making. Regular customers of nuclear data will note that there are few changes to the standard ENDF/B library as compared to past years. This was because we have been processing and testing all the beta versions of ENDF/B-VIII.0. During this processing and testing we have reported and fixed many of the issues that would have been a problem. We continue to work with the broader nuclear data community to provide the best nuclear data available.

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A Elementals

The scripts that were used to calculate the natural elements can be found in a git repository hosted here: <https://xcp-stash.lanl.gov/projects/NDT/repos/elementals/>. The isotopic weights used to create the elementals can be found in Table 6

Table 6: Isotopic weights used to calculate the elemental values.

Elemental	Isotopic ZA	Weight
1000	1001	0.999 850 00
	1002	0.000 150 00
2000	2003	0.000 001 37
	2004	0.999 998 63
3000	3006	0.075 900 00
	3007	0.924 100 00
4000	4009	1.000 000 00
5000	5010	0.198 000 00
	5011	0.802 000 00
6000	6012	0.988 900 00
	6013	0.011 100 00
7000	7014	0.996 340 00
	7015	0.003 660 00
8000	8016	0.997 620 00
	8017	0.000 380 00
	8018	0.002 000 00
9000	9019	1.000 000 00
10000	10020	0.904 800 00
	10021	0.002 700 00
	10022	0.092 500 00
11000	11023	1.000 000 00
12000	12024	0.789 900 00
	12025	0.100 000 00
	12026	0.110 100 00
13000	13027	1.000 000 00
14000	14028	0.922 300 00
	14029	0.046 830 00
	14030	0.030 870 00
15000	15031	1.000 000 00
16000	16032	0.950 200 00

Continued on next page

Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
	16033	0.007 500 00
	16034	0.042 100 00
	16036	0.000 200 00
17000	17035	0.757 700 00
	17037	0.242 300 00
18000	18036	0.003 365 00
	18038	0.000 632 00
	18040	0.996 003 00
19000	19039	0.932 581 00
	19040	0.000 117 00
	19041	0.067 302 00
20000	20040	0.969 410 00
	20042	0.006 470 00
	20043	0.001 350 00
	20044	0.020 860 00
	20046	0.000 040 00
	20048	0.001 870 00
21000	21045	1.000 000 00
22000	22046	0.082 500 00
	22047	0.074 400 00
	22048	0.737 200 00
	22049	0.054 100 00
	22050	0.051 800 00
23000	23050	0.002 500 00
	23051	0.997 500 00
24000	24050	0.043 450 00
	24052	0.837 890 00
	24053	0.095 010 00
	24054	0.023 650 00
25000	25055	1.000 000 00
26000	26054	0.058 450 00
	26056	0.917 540 00
	26057	0.021 190 00
	26058	0.002 820 00
27000	27059	1.000 000 00
28000	28058	0.680 770 00
	28060	0.262 230 00

Continued on next page

Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
	28061	0.011 400 00
	28062	0.036 340 00
	28064	0.009 260 00
29000	29063	0.691 700 00
	29065	0.308 300 00
30000	30064	0.486 300 00
	30066	0.279 000 00
	30067	0.041 000 00
	30068	0.187 500 00
	30070	0.006 200 00
31000	31069	0.601 080 00
	31071	0.398 920 00
32000	32070	0.203 700 00
	32072	0.273 100 00
	32073	0.077 600 00
	32074	0.367 300 00
	32076	0.078 300 00
33000	33075	1.000 000 00
34000	34074	0.008 900 00
	34076	0.093 700 00
	34077	0.076 300 00
	34078	0.237 700 00
	34080	0.496 100 00
	34082	0.087 300 00
35000	35079	0.506 900 00
	35081	0.493 100 00
36000	36078	0.003 500 00
	36080	0.022 800 00
	36082	0.115 800 00
	36083	0.114 900 00
	36084	0.570 000 00
	36086	0.173 000 00
37000	37085	0.721 700 00
38000	38084	0.005 600 00
	38086	0.098 600 00
	38087	0.070 000 00
	38088	0.825 800 00

Continued on next page

Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
39000	39089	1.000 000 00
40000	40090	0.514 500 00
	40091	0.112 200 00
	40092	0.171 500 00
	40094	0.173 800 00
	40096	0.028 000 00
41000	41093	1.000 000 00
42000	42092	0.148 400 00
	42094	0.092 500 00
	42095	0.159 200 00
	42096	0.166 800 00
	42097	0.095 500 00
	42098	0.241 300 00
	42100	0.096 300 00
44000	44096	0.055 400 00
	44098	0.018 700 00
	44099	0.127 600 00
	44100	0.126 000 00
	44101	0.170 600 00
	44102	0.315 500 00
	44104	0.186 200 00
45000	45103	1.000 000 00
46000	46102	0.010 200 00
	46104	0.111 400 00
	46105	0.223 300 00
	46106	0.273 300 00
	46108	0.264 600 00
	46110	0.117 200 00
47000	47107	0.518 390 00
	47109	0.481 610 00
48000	48106	0.012 500 00
	48108	0.008 900 00
	48110	0.124 900 00
	48111	0.128 000 00
	48112	0.241 300 00
	48113	0.122 200 00
	48114	0.287 300 00
	48116	0.074 900 00

Continued on next page

Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
49000	49113	0.042 900 00
	49115	0.957 100 00
50000	50112	0.009 700 00
	50114	0.006 600 00
	50115	0.003 400 00
	50116	0.145 400 00
	50117	0.076 800 00
	50118	0.242 200 00
	50119	0.085 900 00
	50120	0.325 800 00
	50122	0.046 300 00
	50124	0.057 900 00
51000	51121	0.572 100 00
	51123	0.427 900 00
52000	52120	0.000 900 00
	52122	0.025 500 00
	52123	0.008 900 00
	52124	0.047 400 00
	52125	0.070 700 00
	52126	0.188 400 00
	52128	0.317 400 00
	52130	0.340 800 00
53000	53127	1.000 000 00
54000	54124	0.000 900 00
	54126	0.000 900 00
	54128	0.019 200 00
	54129	0.264 400 00
	54130	0.040 800 00
	54131	0.211 800 00
	54132	0.268 900 00
	54134	0.104 400 00
	54136	0.088 700 00
55000	55133	1.000 000 00
56000	56130	0.001 060 00
	56132	0.001 010 00
	56134	0.024 170 00
	56135	0.065 920 00
	56136	0.078 540 00
	56137	0.112 320 00

Continued on next page

Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
	56138	0.716 980 00
57000	57139	0.999 100 00
58000	58136	0.001 850 00
	58138	0.002 510 00
	58140	0.884 500 00
	58142	0.111 140 00
59000	59141	1.000 000 00
60000	60142	0.272 000 00
	60143	0.122 000 00
	60145	0.083 000 00
	60146	0.172 000 00
	60148	0.057 000 00
	60150	0.056 000 00
62000	62144	0.030 700 00
	62147	0.149 900 00
	62149	0.138 200 00
	62150	0.073 800 00
	62152	0.267 500 00
	62154	0.227 500 00
63000	63151	0.478 100 00
	63153	0.521 900 00
64000	64152	0.002 000 00
	64154	0.021 800 00
	64155	0.148 000 00
	64156	0.204 700 00
	64157	0.156 500 00
	64158	0.248 400 00
	64160	0.218 600 00
65000	65159	1.000 000 00
66000	66156	0.000 600 00
	66158	0.001 000 00
	66160	0.023 400 00
	66161	0.189 100 00
	66162	0.255 100 00
	66163	0.249 000 00
	66164	0.281 800 00
67000	67165	1.000 000 00

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Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
68000	68162	0.001 390 00
	68164	0.016 010 00
	68166	0.335 030 00
	68167	0.228 690 00
	68168	0.269 780 00
	68170	0.149 100 00
69000	69169	1.000 000 00
70000	70168	0.001 300 00
	70170	0.030 400 00
	70171	0.142 800 00
	70172	0.218 300 00
	70173	0.161 300 00
	70174	0.318 300 00
	70176	0.127 600 00
71000	71175	0.974 100 00
72000	72174	0.001 600 00
	72176	0.052 600 00
	72177	0.186 000 00
	72178	0.272 800 00
	72179	0.136 200 00
	72180	0.350 800 00
73000	73181	0.999 880 00
74000	74180	0.001 200 00
	74182	0.265 000 00
	74183	0.143 100 00
	74184	0.306 400 00
	74186	0.284 300 00
75000	75185	0.374 000 00
76000	76184	0.000 200 00
	76186	0.015 900 00
	76187	0.016 000 00
	76188	0.132 900 00
	76189	0.162 100 00
	76190	0.263 600 00
	76192	0.409 300 00
77000	77191	0.373 000 00
	77193	0.627 000 00

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Table 6: Isotopic weights used to calculate the elemental values (*continued*).

Elemental	Isotopic ZA	Weight
78000	78192	0.007 820 00
	78194	0.329 670 00
	78195	0.338 320 00
	78196	0.252 420 00
	78198	0.071 630 00
79000	79197	1.000 000 00
80000	80196	0.001 500 00
	80198	0.099 700 00
	80199	0.168 700 00
	80200	0.231 000 00
	80201	0.131 800 00
	80202	0.298 600 00
	80204	0.068 700 00
81000	81203	0.295 240 00
	81205	0.704 760 00
82000	82204	0.014 000 00
	82206	0.241 000 00
	82207	0.221 000 00
	82208	0.524 000 00
83000	83209	1.000 000 00

B Archive

The files used to generate these libraries—and all the beta libraries in preparation—have been archived in HPSS here: </hpss/nucldata/sn/Lib80x>