LA-UR-18-24034
Approved for public release; distribution is unlimited.

Title: Release of ENDF/B-VIII.0-Based ACE Data Files

Author(s): Conlin, Jeremy Lloyd
Haeck, Wim
Neudecker, Denise
Parsons, Donald Kent
White, Morgan Curtis

Intended for: Report

Issued: 2018-05-09

Disclaimer:
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Release of ENDF/B-VIII.0-Based ACE Data Files

Jeremy Lloyd Conlin*, Wim Haeck, Denise Neudecker, D. Kent Parsons, and Morgan C. White

Nuclear Data Team, XCP-5
Los Alamos National Laboratory

May 7, 2018

1. Introduction

In February 2018, the National Nuclear Data Center released ENDF/B-VIII.0 [1] in the standard Evaluated Nuclear Data Format (ENDF) [2]. This represents the advances made in nuclear data since the release of ENDF/B-VII.1 [3] in 2011.

The Nuclear Data Team at Los Alamos National Laboratory has processed the ENDF/B-VIII.0 library and has made available a library of ACE data tables at several temperatures for each of the incident neutron ENDF/B files. The library is called Lib80x and is distributed from the website `https://nucleardata.lanl.gov`. The data was processed using NJOY2016.27 [4, 5]; a sample NJOY input deck is given in Appendix A.

The release of the Lib80x library includes all the ENDF/B-VIII.0 incident neutron evaluations processed to the seven temperatures shown in Table 1. These are the same temperatures used for the ENDF/B-VII.1-based library, ENDF71x [6, 7].

1.1. ZA Identifiers

For ENDF/B-VIII.0, 135 incident neutron evaluations were added and one (natural carbon, ZA=6000) was removed. The identifiers—or "names" that uniquely identify a specific data table—contain the ZA of the material. The ZA is calculated as

$$\mathsf{ZA} = Z * 1000 + A, \tag{1a}$$

*Corresponding author `jlconlin@lanl.gov`

Temperature (K)	ZAID Extension	SZAID Extension
293.6	.00c	.800c
600	.01c	.801c
900	.02c	.802c
1200	.03c	.803c
2500	.04c	.804c
0.1	.05c	.805c
250	.06c	.806c

Table 1: Temperatures and extensions for ZAIDs and SZAIDs in Lib80x.

or, for metastable materials

$$\mathsf{ZA} = Z * 1000 + A + 300 + S * 100 \tag{1b}$$

where Z is the atomic number, A is the atomic mass number and S is the excited state number. Thus for ^{1}H, ZA=1001; for ^{56}Fe, ZA=26056; for ^{137m1}Ce, ZA=58537; and for ^{235}U, ZA=92235.

There is an exception to this for ^{242}Am. For historical reasons[1] ZA-95242 is for the first metastable state of ^{242}Am and ZA=95642 is for ground-state ^{242}Am. The ZAs in Lib80x are given in Table 2.

Table 2: ZAs for nuclei included in Lib80x.

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	13426†	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			
26054	26055*	26056	26057	26058	27058	27458†	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

continued...

[1] Prior to ENDF/B-VII.1, only the first excited state of ^{242}Am was available and ZA=95242 was used. We keep this anomaly for historical reasons.

Table 2: ZAs for nuclei included in Lib80x (*continued*).

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	46102	46103*	46104
46105	46106	46107	46108	46109*	46110	47107	47108*	47109	47510†
47111	47112*	47113*	47114*	47115*	47116*	47117*	47518‡	48106	48107*
48108	48109*	48110	48111	48112	48113	48114	48515†	48116	49113
49114*	49115	50112	50113	50114	50115	50116	50117	50118	50119
50120	50521‡	50122	50123	50124	50125	50126	51121	51122*	51123
51124	51125	51126	52120	52121*	52521‡	52122	52123	52124	52125
52126	52527†	52128	52529†	52130	52131*	52531‡	52132	53127	53128*
53129	53130	53131	53132*	53532‡	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*	58537‡	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	61548†
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	67566†	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	75586‡	75187	76184*	76185*	76186*	76187*	76188*	76189*	76190*
76191*	76192*	77191	77192*	77193	77594‡	78190*	78191*	78192*	78193*
78194*	78195*	78196*	78197*	78198*	79197	80196	80197*	80597‡	80198
80199	80200	80201	80202	80203*	80204	81203	81204*	81205	82204
82205*	82206	82207	82208	83209	83610‡	84208*	84209*	84210*	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	93636‡	93237	93238	93239	94236	94237	94238	94239	94240
94241	94242	94243	94244	94245*	94246	95240	95241	95642†	95242

continued...

Table 2: ZAs for nuclei included in Lib80x (*continued*).

95243	95244	95644†	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	99654†	99255	100255				

* New evaluations in ENDF/B-VIII.0.
† Excited state evaluations

1.2. SZAID Identifiers

In keeping with the precedent set with the ENDF71x library [6], we have used the 2.0.1 header format [8, 9] for the ACE data tables that are backwards compatible with the legacy or traditional header. These use an SZAID as the unique identifier which contains an SZA—an expanded ZA—and a three-digit extension. While MCNP cannot (yet) handle an SZA, we still make it available as a unique identifier for the materials in the Lib80x library. An SZA is calculated similarly to an ZA:

$$\mathsf{SZA} = S * 1\,000\,000 + Z * 1000 + A. \tag{2}$$

Like with the ZA, ^{242}Am is an historical exception where SZA=`1095242` is used for the ground-state data and SZA=`95242` is used for the first meta-stable state. The SZAID extensions and their associated temperatures are given in Table 1.

2. Testing the ACE Files

We have performed a number of tests on the processed data to ensure it's quality. We have two main ways of testing the processed ACE files: 1) performing MCNP6 [10] calculations for benchmark models; and 2) running `checkACE` [11], a series of checks on the physics of the nuclear data.

2.1. `checkACE`

`checkACE` is a collection of 10 Fortran routines which read the ACE files prepared by NJOY for MCNP. Common sense testing of data values is performed and anomalous results are reported. These results may be due to problems in the evaluation files, or in the NJOY processing, or in the checking procedures themselves. Follow-up investigation is required to pinpoint the cause of the anomalous results.

We do not document here the specific checks that are performed by `checkACE`; those are reported in *The Rules of CHECKACE – a Suite of Checking Codes for MCNP ACE Cross Section Files* [11]. We do report on the anomalous findings and what we have done to mitigate the errors. Note that for some cases, we don't provide an immediate solution, but do note the issue.

check5 ^{131}Pa and ^{133}Pa values for the number of secondary neutrons produced from `MT=5` that are close to—or larger than—the current MCNP limit of 11 secondary particles. (This is a long-standing issue in the protactinium evaluation files.)

check_heat Several isotopes have a large number of negative kerma/heating values:

- ^{94}Mo
- ^{96}Mo
- ^{97}Mo
- ^{98}Mo
- ^{119m1}Ag
- ^{131m1}Te
- ^{132m1}I
- ^{137m1}Cs
- ^{168}Yb
- ^{170}Yb
- ^{171}Yb
- ^{172}Yb
- ^{173}Yb
- ^{174}Yb
- ^{176}Yb
- ^{194m1}Ir
- ^{197m1}Hg
- ^{208}Po

Negative kerma/heating values indicate a problem with the evaluation and nothing has been done to correct this.

check_ures Only three nuclides had negative cross sections in the probability tables coming out of NJOY: ^{22}Na, ^{36}Ar and ^{106}Cd. These negative cross sections appear because the evaluation of these nuclides has an `LSSF` flag of `0` (`MF=3` contains background cross sections) and all or some of these background cross sections are negative in the unresolved resonance region. When sampling the cross section values from the unresolved resonance parameters, these backgrounds need to be added to the final cross section values. Negative values can therefore occur when the sampled cross section values are small. Because the cross section values are sorted prior to generating the probability bins, these negative cross section bins are often limited to the first few bins of the probability table. These three nuclides were therefore reprocessed without probability tables.

Negative cross sections also appeared in the ^{240}Pu probability tables but this was traced back to an error in the evaluation (the total cross section was smaller than its components, thus leading to an artificial negative background for the total cross section). NJOY2016 was updated to handle such a case by setting the resulting total background to 0.0 when the total cross section appeared to be smaller than its components. More information can be found in *NJOY2016 Updates for ENDF/B-VIII.0* [12].

checknd_n The ACE checking codes also detected non-monotonic CDF values for ^{20}Ne and a negative PDF value for ^{37}Ar. Both nuclides are new to ENDF/B-VIII.0 and were taken from the TENDL libraries. Both problems were solved by correcting the evaluation.

For ^{20}Ne, the issue appeared in the secondary neutron energy-angular distribution from `MF=6`/`MT=22`. NJOY2016 has an option that is switched on by default to smooth the lower energy part of center-of-mass distributions that uses a histogram representation for the outgoing energy with a $\sqrt{E}$ shape. However, NJOY assumes that the first energy value is always 0 eV when doing this. In this case, the first energy value was not 0 eV but 1.457 852 MeV. NJOY therefore added outgoing energy values after this first energy point that were actually smaller than 1.457 852 MeV. This resulted in the appearance of negative CDF values for these added outgoing energy points. This only occurred for

the following incident neutron energies: 7.4 MeV, 8 MeV, 8.5 MeV, 9 MeV and 10 MeV. All other incident energy values used 0 eV as the first outgoing energy point. Because the probability of this first outgoing energy bin was set to 1×10^{-19} in the evaluation, it was decided to correct the evaluation directly by replacing the original outgoing energy of 1.457 852 MeV by 0 eV. This correction has no impact on the actual PDF values of the other outgoing energy bins.

For ^{37}Ar, the issue appeared in the secondary neutron energy-angular distribution from `MF=6`/`MT=5`. For QA purposes, NJOY2016 includes a number of consistency checks which may either inform the user of an issue or even automatically correct data in an ACE file when a problem is detected. One such test is the verification of the maximum outgoing neutron energy to see if it is smaller than the physically possible maximum outgoing energy. If NJOY detects such a problem, NJOY will correct the outgoing energy value to not be higher than the physically possible maximum outgoing energy after which it will renormalise the CDF. Under normal circumstances, the outgoing energy values are only changed by very small fractions. In the case of `MF=6`/`MT=5` of ^{37}Ar, the evaluation included several outgoing energy values with associated probabilities of 1×10^{-16} or lower that were above the physically possible maximum outgoing energy. The differences were of the order of a few to even 10 % in some cases. This leads to a negative CDF value for an incident energy of 160 MeV after the renormalisation of the CDF. Due to the low probability of these outgoing energy values, it was decided to correct the evaluation directly by removing the outgoing energy bins at the end of the distribution for each incident energy value if the associated probability was lower than 1×10^{-16}. As with the correction for ^{20}Ne, this correction has no impact on the actual PDF values of the other outgoing energy bins.

2.2. Benchmark Models

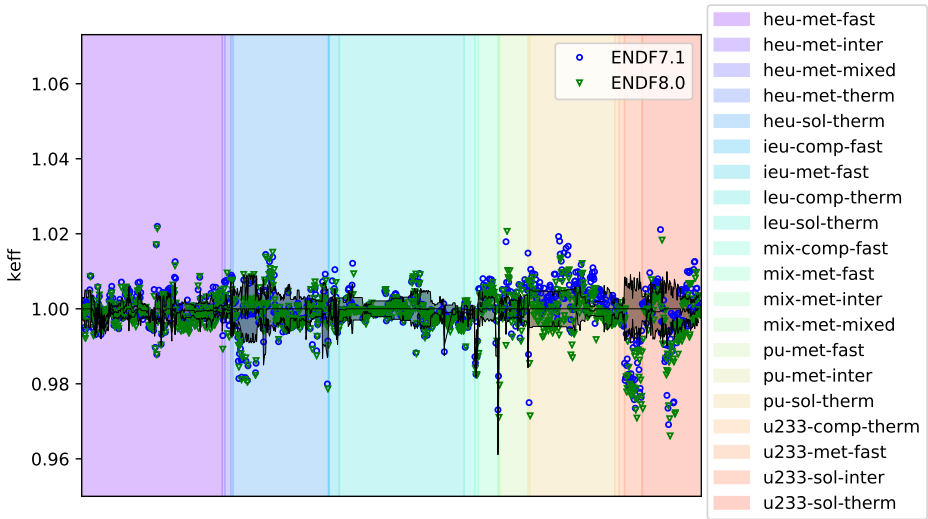
We have performed MCNP calculations for two different kinds of benchmarks: 1. critical benchmarks from the ICSBEP [13] as created by "Skip Kahler" (see [1, Appendix A]); and 2. pulsed sphere calculations.

We don't report on the details of these benchmark models here; additional reports/papers on the analysis are forthcoming. We do show the graphical results of the benchmark calculations in Figure 1, where the calculated k_{eff} values for 1151 benchmark simulations are shown. These are the same benchmark models in [1, Appendix A]. In Figure 1b is shown the ratio of the calculated k_{eff} value to the experimentally measured value.

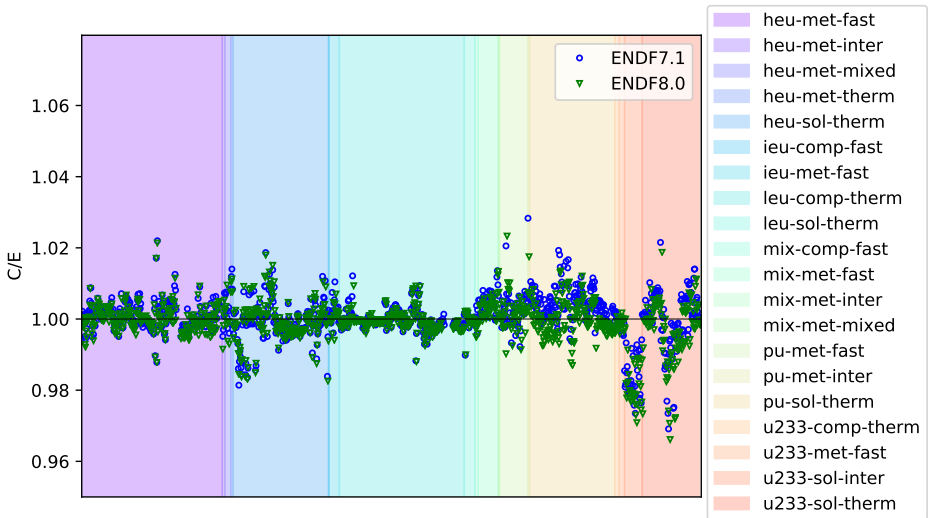
In Figure 2 we show the comparison of pulsed sphere calculations using ENDF/B-VII.1 and ENDF/B-VIII.0-based data libraries. As with the critical benchmarks, we can see that the ENDF/B-VIII.0-based libraries better match—on average—the experimental values than the ENDF/B-VII.1-based library.

3. Changes to NJOY

Each release of the ENDF/B library often results in the introduction of new data formats in the ENDF-6 format. With ENDF/B-VIII.0, which was released in February 2018,

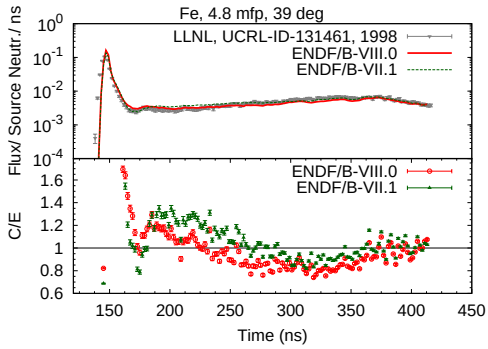


(a) Calculated k_{eff} results for 1151 critical assembly models. The black lines and shaded region shows the experimentally measured value and uncertainty, respectively.

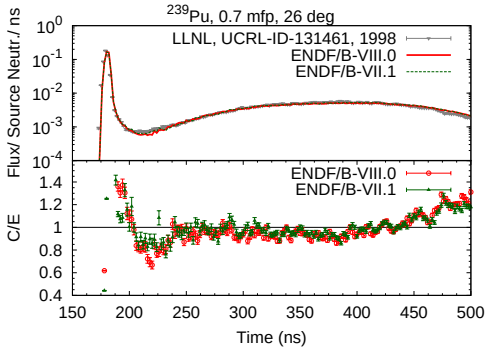


(b) Ratio of calculatd (MCNP) to experimental k_{eff} results.

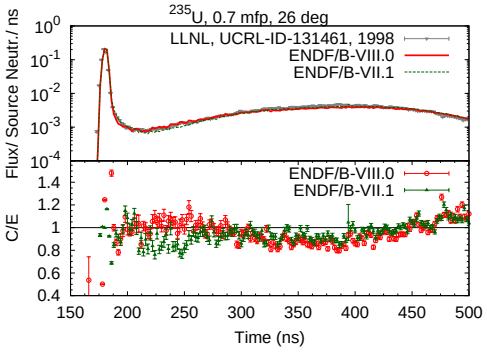
Figure 1: k_{eff} results from the final version of ENDF/B-VIII.0.



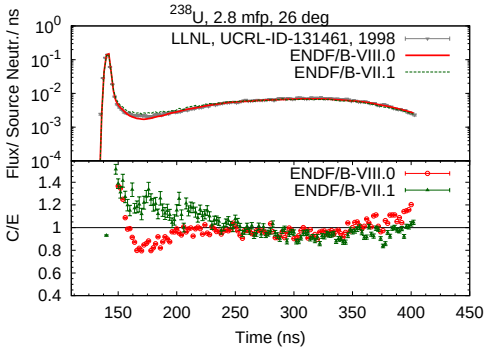
(a) Iron



(b) Pu-239



(c) U-235



(d) U-238

Figure 2: Comparison of measured LLNL pulsed sphere data with ENDF/B-VII.1 and ENDF/B-VIII.0 simulations.

new formats were added for allowing tabulated fission energy release components in the `MF=1/MT=458` section, to allow for sub-actinide fission and non-neutron induced fission in the `MF=8/MT=18` and `MF=10/MT=18` sections, and to add fission neutron and gamma emission probabilities in the `MF=6/MT=18` section [2]. Processing codes must be adapted to ensure that they are capable of using these new data, or at the very least understand the new formats. NJOY2016, the production version of the nuclear data processing code developed at Los Alamos National Laboratory is no exception to this.

In addition to format changes, a new evaluated nuclear data library also tends to push the limits of the processing codes leading to a number of fixes and updates to correct problems that were uncovered while processing the beta releases and final release of ENDF/B-VIII.0:

- Updates to ACER for plot generation and thermal scattering data formatting.
- Updates to ERRORR for covariance processing.
- Updates to LEAPR for generating thermal scattering data.
- Updates to PURR for unresolved resonance probability tables.
- Updates to THERMR for thermal scattering data.
- Integration of an NJOY2012 update file from the IAEA

For more detailed information about the changes made to NJOY2016, please see *NJOY2016 Updates for ENDF/B-VIII.0* [12].

4. Conclusion

The Lib80x library is recommended for use in all Monte Carlo transport calculations. It contains updated nuclear data which is a result of many years of work by researchers from around the world.

References

[1] D.A. Brown et al. "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data". In: *Nuclear Data Sheets* 148 (2018). Special Issue on Nuclear Reaction Data, pp. 1–142. ISSN: 0090-3752. DOI: https://doi.org/10.1016/j.nds.2018.02.001. URL: https://www.sciencedirect.com/science/article/pii/S0090375218300206.

[2] A. Trkov, M. Herman, and D. A. Brown. *ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data Files ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII*. Tech. rep. BNL-203218-2018-INRE. National Nuclear Data Center, Brookhaven National Laboratory, Feb. 2018.

[3] M.B. Chadwick et al. "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data". In: *Nuclear Data Sheets* 112.12 (2011), pp. 2887–2996. ISSN: 0090-3752. DOI: 10.1016/j.nds.2011.11.002. URL: http://www.sciencedirect.com/science/article/pii/S009037521100113X.

[4] A. C. Kahler et al. *NJOY2016*. 2016. URL: https://github.com/njoy/NJOY2016 (visited on 2016).

[5] R. E. MacFarlane et al. *The NJOY Nuclear Data Processing System, Version 2016*. Ed. by A. C. Kahler. LA-UR-17-20093. Los Alamos National Laboratory. Dec. 2016. URL: https://github.com/njoy/NJOY2016-manual.

[6] Jeremy Lloyd Conlin et al. *Continuous Energy Neutron Cross Section Data Tables Based upon ENDF/B-VII.1*. Tech. rep. LA-UR-13-20137. Los Alamos National Laboratory, Feb. 2013.

[7] Jeremy Lloyd Conlin et al. "Release of ENDF/B-VII.1-based Continuous Energy Neutron Cross Section Data Tables for MCNP". In: *Transactions of the American Nuclear Socity*. LA-UR-13-20240. Atlanta, Georgia: American Nuclear Society, June 2013.

[8] Jeremy Lloyd Conlin et al. *Version 2.0.0 of ACE Tables Header Format*. Tech. rep. LA-UR-12-25177. Los Alamos National Laboratory, Sept. 2012.

[9] Mark G. Gray. *ACE Table Header Format Version 2.0.1*. Memo XCP-5:15-054. Los Alamos National Laboratory, Sept. 2015.

[10] T. Goorley et al. "Initial MCNP6 Release Overview". English. In: *Nuclear Technology* 180.3, SI (DEC 2012), 298–315. ISSN: 0029-5450.

[11] D. Kent Parsons. *The Rules of CHECKACE – a Suite of Checking Codes for MCNP ACE Cross Section Files*. Memo XCP-5:15-032. Los Alamos National Laboratory, Apr. 2015.

[12] W. Haeck et al. *NJOY2016 Updates for ENDF/B-VIII.0*. Tech. rep. LA-UR-18-22676. Los Alamos National Laboratory, 2018.

[13] J. Blair Briggs. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. September 2013. Nuclear Energy Agency (AEN/NEA), 2013.

A. Typical NJOY Input Deck

The Nuclear Data Team at LANL typically produces ACE files using a few NJOY steps instead of one large input deck. The steps are:

1. reconstruct the resonances,
2. Doppler broaden to the appropriate temperature, and
3. create an ACE file.

Each step has its own input deck, examples of which are given below for ^{235}U. You will note that there are multiple NJOY modules called at each step in the processing.

Resonance Reconstruction

```
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 /
stop

```

Doppler Broadening, KERMA, and Gas Production

```
moder
  -31 -41 /
broadr
  -30 -31 -32 /
  9228 1 0 0 0.0 /
  0.001 1000000.0 0.01 5.0000000000000004e-08 /
  293.6
  0 /
broadr
  -30 -41 -42 /
  9228 1 0 0 0.0 /
  0.001 -10000000.0 0.01 5.0000000000000004e-08 /
  293.6
  0 /
heatr
  -30 -32 -33 /
  9228 3 0 0 0 2 /
  442
  443
  444
heatr
  -30 -42 -43 /
  9228 3 0 0 0 2 /
  442
  443
  444
gaspr
  -30 -33 -34 /
gaspr
  -30 -43 -44 /
thermr
  0 -34 -35 /
  0 9228 16 1 1 0 0 1 221 2 /
  293.6 /
  0.001 10.0 /
thermr
  0 -44 -45 /
  0 9228 16 1 1 0 0 1 221 2 /
  293.6 /
  0.001 10.0 /
moder
  -35 22 /
moder
  -45 23 /
stop
```

ACE Creation

```
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 Lib80x (jlconlin)  Ref. see jlconlin (ref 01/29/2018 07:54)' /
  9228 293.6 /
  1 1 /
  /
acer
  0 23 0 25 26 /
  7 1 1 0.800000 /
  'U235 Lib80x (jlconlin)  Ref. see jlconlin (ref 01/29/2018 07:54)' /
stop

```