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ENDF70: A CONTINUOUS-ENERGY MCNP NEUTRON DATA LIBRARY BASED ON ENDF/B-VII.0

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Following the release of ENDF/B-VII.0 evaluations, an ACE-formatted continuous-energy neutron data library called ENDF70 for MCNP has been produced at Los Alamos National Laboratory. This new library contains data for 389 isotopes and three elements at five temperatures: 293.6, 600, 900, 1200, and 2500 K. It can be obtained as part of the MCNP5 1.50 release. The new library was created using ENDF/B-VII.0 neutron evaluations and primarily Version 248 of NJOY99. A processing script was created that set up the input files for NJOY and employed checking codes to test the content of the processed data. A sample MCNP run was performed for each isotope and temperature, and cross sections for each isotope were plotted to make sure there were no major problems. The processed ACE libraries did not always pass all quality assurance tests. For example, energy-balance problems were identified for several evaluations having negative heating numbers or inconsistencies between total and partial heating. Similarly, some problems were found with unresolved resonance probability tables resulting in probability tables being excluded from the final library for several materials. Certain evaluations were modified and re-processed as a result of the quality assurance tests, and some data points in the final ACE files were changed because they were too small or had other problems. The new ENDF70 library provides MCNP users with the latest ENDF/B data available. This collection of data includes a larger range of isotopes and temperatures than previously released, which will be beneficial in numerous applications. The upgrades included as part of ENDF/B-VII.0 and hence ENDF70 should improve calculations.

I. INTRODUCTION

The ENDF/B-VII.0 nuclear data evaluations contain neutron cross sections for 390 isotopes and 3 elements.[1] All evaluations with the exception of ^{7}Be, which was incomplete, have been processed into ACE format at five different temperatures: 293.6, 600, 900, 1200, and 2500 K to create the ENDF70 library for MCNP. Most of the processing was done using NJOY99[2] Version 248. Several pre- and post-processing scripts and quality assurance checking codes were utilized as well. The ENDF70 neutron library was broken into eleven separate files of less than 900 MB each and will be compressed and released with MCNP5 1.50. The major changes to ENDF70 not present in a predecessor MCNP library named ENDF66[3] were more temperatures, inclusion of substantially more nuclides including metastable states, and a new XSDIR file with atomic weights for the new nuclides. All advanced physics features found in ENDF66, including delayed neutron spectra, tabulated angular distributions, unresolved resonance probability tables, and charge-particle production data, have also been provided in ENDF70.

II. BACKGROUND

Nuclear data are distributed with the MCNP package; thus are used extensively worldwide. The release of the ENDF66 neutron library based upon data from ENDF/B-VI.6 involved many quality assurance tests to make sure the best data possible were released. Checking codes were written and each evaluation was plotted and tested in MCNP to make sure no major problems existed. The same rigorous procedure was employed for release of the ENDF70 library based on ENDF/B-VII.0 data. During the processing of the ENDF66 library, some limitations of NJOY99 Version 50 were found that related to unresolved resonance tables (the PURR module) and the ability to process delayed neutron data. These issues required post-processing of NJOY data to create the tables released as part of ENDF66. All of these issues have been resolved in version 248 of NJOY, thus eliminating the need for post-processing for ENDF70.

III. NEW FEATURES OF ENDF70

There are numerous factors that were considered when processing the ENDF70 library, including providing more temperature-dependent data, inclusion of nuclides in metastable states, and the addition of new isotopes that were not previously processed. The next several sections discuss these features in more detail.

III.A. Temperature-Dependence

The temperature-dependent cross sections in ENDF70 have ZAID identifiers of .70c, .71c, .72c, .73c, and .74c respectively (see Table I). The purpose of providing more intermediate temperatures than previously released is to make reactor-type calculations easier both directly and with the use of the Doppler code[4] released with MCNP5 1.50. Given pre-existing ACE-formatted libraries, Doppler prepares cross sections for any temperature greater than a temperature in an existing library. However, Doppler interpolates values for the thermal scattering and unresolved-resonance probability tables and can do so more accurately with an "upper" and "lower" bound of the temperature range. Having multiple temperatures available aids users in obtaining more accurate results at temperatures of interest.

Table I. Mapping of ZAID Identifiers to Temperatures

Identifier	Temperature (K)
*.70c	293.6
*.71c	600
*.72c	900
*.73c	1200
*.74c	2500

III.B. Inclusion of All Targets Including Metastable States

Previous MCNP libraries, such as ENDF66, did not include data for all the materials available in the corresponding evaluated data base. For ENDF70, we decided to process and distribute MCNP data sets for all materials evaluated in ENDF/B-VII.0. Subsequently, we discarded ^{7}Be, which is an incomplete evaluation. Nevertheless, we do include data for the remaining 392 materials comprising ENDF/B-VII.0, which is a substantial increase relative to previous MCNP libraries.

Another major addition to ENDF70 is the inclusion of data for nine isomers. The ZAID identifier for an isomer needs to be distinct from that for the ground state. As such we have chosen to use ZAID identifiers for nuclides in metastable states that involve unrealistic atomic mass numbers so they will not only be different from the ground state but also stand out to users. The atomic mass for the ZAID of a nuclide in a metastable state can be calculated using Equation 1.

$$ZAID_m = (ZAID + 300) + (m*100) \quad [1]$$

Where: $ZAID_m$ is the metastable isomer ZAID
ZAID is the ground-state ZAID
m is the excited state (i.e. m=0,1,2,3…)

There is one exception to this ZAID rule for isomers: ^{242m}Am. MCNP data libraries including ^{242m}Am have been distributed for some time, and the identifier for the metastable state has always been 95242. Previous to this library, MCNP data for the ground state of ^{242}Am have not been distributed. To avoid backwards-compatibility issues, we have an unusual identifier for the ground state of ^{242}Am: 95642. The ZAID of ^{242m}Am remains as 95242. Table II contains a list of nuclides for which metastable state data are available in ENDF70 (along with the corresponding ground state, if available) and their ZAID identifiers.

Table II. Nuclides with Metastable States in ENDF70

Isotope	ZAID
^{58}Co	27058
^{58m}Co	27458
^{110m}Ag	47510
^{115m}Cd	48515
^{127m}Te	52527
^{129m}Te	52529
^{148}Pm	61148
^{148m}Pm	61548
^{166m}Ho	67566
^{242}Am	95642
^{242m}Am	95242
^{244}Am	95244
^{244m}Am	95644

III.C. Changes to XSDIR

MCNP must have access to atomic weights for any material in a problem. The file "xsdir" provides information about the available cross section files, and also provides atomic weights (actually atomic-weight ratios) for all available isotopes. Because cross sections for many isotopes are newly available on ENDF70, atomic weights had to be added to xsdir.

Because we were adding a large number of new isotopes to the atomic weight ratio section of xsdir, a decision was made to completely update the section to include values from the most recent compilation.[5] As a result, the xsdir file distributed with MCNP5 1.50 not only provides new atomic weight ratios for previously-unavailable isotopes such as ^{133}Ba, it also provides updated (relative to previous xsdir) atomic weight ratios for previously-available isotopes such as ^{235}U.

IV. METHOD

All processing of ENDF/B-VII data was done on a LINUX machine using Version 248 of NJOY (the sole exception is ^{1}H, for which update 271 was also applied). The modules MODER, RECONR, BROADR, HEATR, PURR, THERMR, and GASPR were used to create PENDF files. The module ACER was then used to create ACE files at each temperature and to perform consistency checking. Most of the modules are common for ACE file processing; the THERMR module was included to avoid some photon-production sum issues found by the consistency checking.

Pre- and post-processors were developed to create the input files for NJOY and to run additional checking scripts on the resulting ACE-formatted data. The same checking codes that analyzed the data in ENDF66 were used for ENDF70 and included: CHECK0, CHECK5, CHECKND, CHECKND_NEUT, CHECK61, CHECK_HEAT, CHECK_ISO, CHECKTHRESH, CHECK_URES, CHECKXS, and CHECK_LOWNUM.PL.[6] The resulting ACE files were also used in a simple MCNP run with neutron and photon transport in a small sphere of material. This test was run separately for each nuclide and temperature to assure no significant problems existed with reading in and using the data in MCNP. Additionally, each isotope was plotted using the program XSPLOT2 to assure no major problems were present in the resulting cross sections.

V. RESULTS

The checking process identified several issues with the processing or with the evaluations. Processing issues often resulted in updates to NJOY. In addition, some changes to the evaluations and some changes to the resulting ACE files were made. Other problems noted by the checking codes still exist but were considered insignificant.

V.A. Evaluation Changes

Evaluations were modified for the following isotopes: ^{1}H, ^{45}Sc, ^{89}Y, ^{96}Zr, ^{97}Mo, ^{242}Am (ground state), and ^{242m}Am. These changes are briefly described below.

^{1}H: The value for the energy of the photon from radiative capture did not take into account the recoil of the nucleus and was modified to 2.2233 from 2.2246 MeV.

^{45}Sc: The secondary distribution for photons (MF=13, MT=3) did not have a zero point at the threshold. Additionally, the evaluation had the incorrect reference frame specified for angular distributions of (n,2n), (n,n*)a, (n,n*)p, and (n,n*c). We made changes to the evaluation and re-processed.

^{89}Y: Negative cross sections for MT=91 from 1.7 to 4.5 MeV were modified to be the difference between MT 4 (total inelastic) and the sum of MT's 51-90 (partial inelastic) reactions.

^{96}Zr and ^{97}Mo: NJOY's CONSIS module identified errors in several MF=6 Law=44 "r" values that were subsequently changed from 0.999999e+1 to 0.999999e+0.

^{242}Am (ground): The angular distribution for fission was missing, so we inserted an isotropic MF=4, MT=18 section.

^{242m}Am: The inelastic cross sections (MT 4, 51, 52, 53, and 54) contained values of zero between 50 and 65 keV, whereas values above and below were non-zero. The cross sections below 100 keV were smoothed out by the evaluator.

V.B. Modifications to the ACE file Resulting from a Checking Code

One of the checking codes checks to see if any negative probability density functions exist and fixes them if so. The only one found during the processing of neutron ENDF/B-VII.0 data was ^{153}Eu (MF=6, MT=91). The negative pdf's were set to 0.0 and the distributions were renormalized in the corrected ACE file. Changes to the ACE files for seven isotopes were also made because they contained exponents less than or equal to e-37: ^{16}O, ^{40}Ca, ^{42}Ca, ^{43}Ca, ^{44}Ca, ^{46}Ca, and ^{204}Pb. The exponents were simply changed to e-35. Finally, one instance of a leading non-zero threshold photon-production cross section value was found for the isotope ^{10}B (MCNP MT=103004). That value was changed to zero and the total photon production cross section at that energy was decremented accordingly.

V.C. Heating (Energy-Balance) Problems

One of the checking codes compares the sum of the partial heating numbers to the total heating reported by NJOY. Some anomalies were found. For example, there were cases where the sum of the partials was greater than the total. The checking code also found some cases of negative heating numbers. Such anomalies are indicative of energy-balance problems in the original evaluations; we report them so users are aware of the issues, but there is nothing that can be done in processing to correct the problems. The isotopes for which these problems occur (with bolded values representing isotopes with negative heating numbers) are:

^{47}Ti, ^{48}Ti, ^{49}Ti, ^{74}As, **^{92}Mo**, **^{94}Mo,** **^{96}Mo**, **^{97}Mo**, **^{98}Mo**, ^{101}Ru, ^{105}Pd, ^{113}Sn, ^{131}Xe, ^{133}Ba, **^{143}Ce**, **^{145}Nd,** **^{147}Nd,** ^{148}Nd, ^{150}Nd, **^{147}Sm**, ^{148}Sm, **^{149}Sm**, **^{151}Sm,** **^{153}Gd**, ^{154}Gd, **^{155}Gd**, ^{156}Gd, ^{157}Gd, ^{191}Ir, and ^{208}Pb.

Note that Versions 115-224 of NJOY99 had a flaw that resulted in incorrect calculation of heating numbers in some cases. During early testing of the ENDF/B-VII data, several heating problems were identified and substantial upgrades were made to NJOY to correct them by Version 248.

V.D. Unresolved Resonance Range Issues

Evaluated data in the unresolved resonance range can sometimes be difficult to process into useful and self-consistent probability tables. Despite several improvements to NJOY, we still found a number of isotopes for which some partial cross sections in the probability tables are not summing up to the totals (within 5%) and/or there are negative heating values. We have not yet had time to determine whether these issues are caused by the evaluations or the processing methods. Thus, probability tables have been excluded (i.e. NJOY was run without PURR) for the following isotopes:

^{22}Na, ^{36}Ar, ^{38}Ar, ^{74}As, ^{79}Se, ^{82}Kr, ^{90}Zr, ^{94}Nb, ^{95}Nb, ^{99}Mo, ^{106}Cd, ^{123}Sn, ^{126}Sn, ^{125}Sb, ^{131}I, ^{136}Cs, ^{139}Ce, ^{143}Pr, ^{144}Nd, ^{148}Pm, ^{151}Pm, ^{153}Sm, ^{152}Eu, ^{153}Eu, ^{154}Eu, ^{155}Eu, ^{156}Dy, ^{158}Dy, ^{181}Ta, ^{252}Cf, ^{253}Cf, and ^{253}Es.

V.E. Final ENDF70 Library

The total size of the new type 1 (i.e. uncompressed) neutron data is approximately 8.8 GB. Compressed, it comprises about 380 MB. The data are broken into eleven different files distinguished by atomic number (Z). Table III lists which elements/isotopes are contained in each data file. The light elements are contained in endf70a, uranium, neptunium and plutonium in endf70j, and other actinides in endf70k. Intermediate-mass structural materials, fission products, and heavy non- actinides are contained in endf70b through endf70i.

Table III. List of Contents in Each ENDF70 file

File	Elements	Z numbers
endf70a	H, He, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V	1 through 23
endf70b	Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge	24 through 32
endf70c	As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo	33 through 42
endf70d	Tc, Ru, Rh, Pd, Ag, Cd	43 through 48
endf70e	In, Sn, Sb, Te, I	49 through 53
endf70f	Xe, Cs, Ba, La, Ce, Pr	54 through 59
endf70g	Nd, Pm, Sm, Eu	60 through 63
endf70h	Gd, Tb, Dy, Ho, Er	64 through 68
endf70i	Lu, Hf, Ta, W, Re, Ir, Au, Hg, Pb, Bi	71 through 83
endf70j	U, Np, Pu	92 through 94
endf70k	Ra, Ac, Th, Pa, Am, Cm, Bk, Cf, Es, Fm	88 through 91 95 through 100

The wide range of fission products now available should help users avoid the need to lump fission products together.

VI. CONCLUSIONS

In summary, the new MCNP neutron library ENDF70 offers more variety in the number of temperatures (5) and available isotopes (392) than in the past. Significant effort was devoted to utilizing checking codes and other testing to assure the quality of ENDF70. The resulting data takes up more storage than in the past but provides improved cross sections for numerous calculations. These data libraries should benefit many users and will be released with MCNP5 1.50.

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