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# YUMMY: THE YUCCA MOUNTAIN MCNP-LIBRARY

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## ABSTRACT

Pointwise libraries provided with the MCNP code contain neutron data for a limited number of temperatures. However, it is important to have the option of using data from a wide range of temperatures for transport calculations. For this purpose, a multi-temperature, ACE-format neutron library was generated for 134 nuclides, as requested by Yucca Mountain Project (YMP) staff. The library is referred to as YUMMY (YUcca Mountain MCNP-librarY). The neutron cross-section data are based on ENDF/B-V or ENDF/B-VI evaluations that were requested by YMP staff. This document provides the details of the new library and its use in criticality safety benchmark problems, a pressurized water reactor design, and waste package models in MCNP4C.

# 1. INTRODUCTION

The Oak Ridge National Laboratory (ORNL) was tasked by the Yucca Mountain Project (YMP) to generate a multi-temperature cross-section library for the purpose of investigating the impact of temperature perturbations on system reactivity. ORNL was tasked to generate ACE format cross-sections for the Monte Carlo N-Particle (MCNP)[1] transport code for 138 nuclides, based on ENDF/B-V, ENDF/B-VI, Los Alamos National Laboratory (LANL) or Lawrence Livermore National Laboratory (LLNL) evaluations. Because evaluations from LANL and LLNL were unavailable, cross-sections were generated based on either ENDF/B-V or ENDF/B-VI data. Among the non-ENDF/B requested isotopes, evaluations did not exist for four of the isotopes and therefore were not processed. As a result, cross-sections for 134 isotopes were processed for seven temperatures, including 0, 294, 373.15, 423.15, 473.15, 523.15, and 587 K, using NJOY99.90.[2] The new library is referred to as YUMMY (<u>YU</u>cca <u>M</u>ountain <u>M</u>CNP-librar<u>Y</u>).

In Section 2, the new library generation is described. Section 3 describes the testing of the continuous-energy cross-section data generated by NJOY using comparisons with AMPX-2000[3] generated data. In Section 4, the new library is applied to criticality safety benchmark cases, as well as pressurized water reactor (PWR) models and PWR and boiling water reactor (BWR) waste package designs in MCNP4C. Finally, Section 5 presents the summary of this work.

# 2. THE TEMPERATURE-DEPENDENT LIBRARY DEVELOPMENT

YMP provided ORNL with a list of 138 nuclides to be processed to generate a pointwise, ACE-format multi-temperature cross-section library. A list of the requested nuclides is provided in Appendix A. For each nuclide, YMP identified the specific evaluation source needed for the cross-section library. Of the evaluation sources, 122 are standard ENDF/B-V or ENDF/B-VI evaluations; however, 16 of the requested evaluation sources are non-standard ENDF/B evaluations. These non-standard evaluations are internal evaluations that were developed at either LANL or LLNL. The non-standard evaluations are not distributed through the National Nuclear Data Center at Brookhaven National Laboratory. Consequently, the 16 non-standard evaluations are not readily available for distribution. Therefore, the missing internal evaluations were replaced with the latest ENDF/B-VI evaluations through Release 7. If a corresponding ENDF/B-VI evaluation did not exist, the appropriate ENDF/B-V evaluation was substituted for the evaluation source.

Using the list of requested nuclides, the entire ENDF/B-V and ENDF/B-VI databases were searched for the evaluation source that matched each nuclide evaluation. The results of the database search are provided in Appendix A. Replacement evaluations for the internal evaluations are also noted in the “comments” column. Note that suitable ENDF/B evaluations are not available to replace three of the requested evaluations for Sn, Np-235, and Np-236. Therefore, these three nuclides have not been processed in the cross-section library development. Additionally, one of the two requested zirconium evaluations developed at LANL was replaced with an ENDF/B-VI evaluation that was the same as that requested for the other zirconium evaluation. Thus, only one zirconium evaluation was processed. As a result, a total 134 nuclides were considered for the new cross-section library.

NJOY input files were prepared for the 134 nuclides listed in Appendix A. The input files were processed with NJOY99.90 on a DEC Alpha XP1000 workstation. Cross-sections were generated for each nuclide at temperatures of 0, 294, 373.15, 423.15, 473.15, 523.15 and 587 K. Sample NJOY input decks are listed in Appendix B for $^{1}$H and $^{238}$U. The input deck for $^{1}$H gives a sample NJOY processing procedure for an isotope that does not have unresolved data processing, as opposed to $^{238}$U, for which unresolved data are processed. The modules used in NJOY for this work are RECONR, BROADR, UNRESR, PURR, THERMR, and ACER. UNRESR and PURR are used only for isotopes that have unresolved data. The RECONR module reconstructs cross-sections in the resonance energy range and generates data that are proper for linear interpolation based on a user-specified tolerance. In BROADR, Doppler-broadening of cross-sections for user-input temperatures is performed. UNRESR and PURR are used for cross-section processing in the unresolved energy range. THERMR processes scattering cross-sections in the thermal energy range. Finally, the ACER module is used to generate two files to be used with MCNP: (1) an ACE-format nuclear data table, and (2) a file that contains a description of the data table.

A nuclear data table contains information for one target isotope, isomer, element, or material. A data table consists of two blocks of data. The first block comprises character information (e.g., nuclide identifier, atomic ratio), counters (e.g., length of the second block of data, number of energies) and pointers (e.g., location of energy table, location of cross-sections). The second block lists the data as a function of energy. The file generated by ACER that gives a description of the data table contains the nuclide identifier (i.e., the table name), atomic weight ratio, name of the cross-section file, access route of the file, file type (ASCII or binary), address (for ASCII files the line number where the table starts, and for binary files the record number of the first record for the table), table length (the total number of words of the second block in the table), record length (applicable for binary files), number of entries per record (applicable for binary files), and temperature. Multiple nuclear data tables concatenated in one file form a data library.

In this work, a total of 938 ASCII ACE-formatted files (134 nuclides at seven different temperatures) were generated by NJOY. These files were grouped based on temperature using the MAKXSF code; i.e., seven files were formed, each file containing data at a particular temperature for 134 nuclides. The names of the libraries formed are ympt0, ympt1, ympt2, ympt3, ympt4, ympt5, and ympt6, corresponding to data generated at 0, 294, 373.15, 423.15, 473.15, 523.15, and 587 K, respectively.

The MAKXSF code is distributed with MCNP for converting cross-section files between formatted sequential-access ASCII and unformatted direct-access binary form. It can also be used to organize data tables for building cross-section libraries. Three inputs are required for MAKXSF:

(1) Nuclear data tables/cross-section libraries
(2) A data directory file

(3) The file “SPECS”

The data directory file consists of three sections. The first section is an optional line that specifies the path where the cross-section data are located; the second section gives atomic weight ratios; and the third section lists the descriptions of the data tables that form the library. The file “SPECS” describes how the new library will be generated; e.g., names of the old and new data directory files, names of the old and new libraries, type of library to be generated (ASCII or binary), and a listing of nuclides that form a library.

The name of the data directory file generated from MAKXSF for the YUMMY ASCII library is “XSDIR1a.” This file is used by MCNP along with the cross-section library. The advantage of using ASCII libraries is their portability between different platforms. However, reading data from a sequential-access ASCII file is more time-consuming compared with reading from a direct-access binary file. Additionally, a binary file is smaller than an ASCII file. The YMP staff requested that the library be provided for use on an HP platform that reads data in big-endian format. Thus the ASCII libraries were converted to binary form using MAKXSF. The binary files were then converted to big-endian format. Depending on the machine on which the big-endian libraries will be placed, the proper data directory file must be used. On the RSICC CD, two data directory files for the binary libraries are provided: XSDIR2b and XSDIR2l. XSDIR2b should be used on machines that read files based on a record length given in bytes (e.g., IBM AIX), and XSDIR2l is for those that read based on a record length given in four-byte (long-word) units (e.g., DEC Alpha). Additionally, in using the big-endian library on platforms that read data in little-endian form, the unit number 34 must be set to big-endian before running MCNP. Unit number 34 corresponds to the logical unit that MCNP uses to open the cross-section library. The big-endian files have been successfully tested on both IBM AIX and DEC Alpha platforms.

## 3. CROSS-SECTION TESTING

A FORTRAN 95 program named RESONATE was developed to read the NJOY-generated cross-sections and perform resonance integral calculations (i.e., for total, elastic scattering, capture, and fission) for each nuclide as a function of temperature. Using a 1/E spectrum as the assumed flux, RESONATE calculates resonance integrals at each temperature and computes the percentage change in the integral as the temperature increases from 373.15 to 587 K. In other words, RESONATE treats the 373.15 K temperature as the base temperature and determines the percentage change in the resonance integral as the temperature increases from the base temperature. The resonance-integral results were performed for 20 different energy ranges from $1 \times 10^{-5}$ eV to 20 MeV. These energy ranges represent 20 bins that are spaced equally in lethargy.

In order to verify the behavior of the NJOY-generated cross-section data, the AMPX-2000 code system was also used to generate temperature-dependent pointwise cross-sections for the 134 nuclides using the same ENDF/B cross-section evaluations. RESONATE was used to perform the same resonance-integral calculations as performed with the NJOY-generated cross-section data.

A FORTRAN 95 program named COMPARE is available to compare the resonance integrals that were calculated with NJOY data with the integrals calculated with AMPX data. COMPARE determines the difference in the resonance integral change as a function of temperature between the two cross-section sets. For example, RESONATE was used to calculate the percentage change in the capture resonance integral as the temperature changes from 373.15 to 423.15 K, using NJOY-generated cross-section data. Likewise, RESONATE was used to calculate the percentage change in the capture integral as the temperature increases from 373.15 to 423.15 K, using the AMPX-generated cross-section data. Subsequently, COMPARE calculated the difference between the NJOY and the AMPX results for the change in the capture integral as a function of temperature. Results show that the behavior of the NJOY- and AMPX-generated resonance integrals agree, to within 1.0% for most of the requested nuclides. There are 11 nuclides where the capture and/or elastic integrals differ by more than 1% between the NJOY- and AMPX- generated integrals. These 11 nuclides are Ca, $^{109}$Ag, $^{152}$Gd, $^{154}$Gd, $^{156}$Gd, $^{160}$Gd, Pb, $^{232}$Th, $^{234}$U, $^{237}$Np, and $^{243}$Am. The differences are attributed to differences in the processing methodology between AMPX and NJOY. The differences do not indicate technical problems with the NJOY-generated data. Therefore, the temperature-dependent MCNP cross-section data are acceptable for use in radiation transport calculations.

## 4. APPLICATION OF THE NEW LIBRARY

The new cross-section library, YUMMY, was used in MCNP4C for a criticality safety benchmark problem obtained from the International Handbook of Evaluated Criticality Safety Benchmark Experiments.[4] The problem identification name is LEU-COMP-THERM-003; it contains 23 critical configurations of water-moderated low-enriched uranium-oxide fuel rods in square pitched arrays. The multiplication factor was computed for the 23 configurations using libraries generated at the aforementioned six temperatures ranging from 294 to 587 K. For the verification of the new multi-temperature library, cross-section libraries distributed with MCNP4C were also used to compute the multiplication factors. The library distributed with MCNP4C will hereafter be referred to as the “MCNP4C original library.” The new library and the MCNP4C original library were compared at 294 K. The statistical uncertainties in the multiplication factors for all cases were less than 0.2%. Table 4.1 gives multiplication factors predicted by MCNP4C, and Table 4.2 presents differences between the MCNP4C original library and the new library in per-cent-mille (pcm).

The YUMMY and MCNP4C original libraries are generally in good agreement. However, in some cases, large discrepancies occur; e.g., in cases 1, 14, and 19, differences of 629, 506, and 815 pcm, respectively, are observed. These discrepancies result from the different versions and options (e.g., tolerances) used in NJOY to generate the two libraries. To examine the effect of different NJOY versions on results, cross-sections were generated from NJOY version 99.81 with the same input decks prepared for NJOY version 99.90 and were used in the benchmark cases. The differences in results obtained using NJOY versions 81 and 90 are anticipated to be based on an update in PURR involving changes in the sampling scheme and binning logic. These results are included in Tables 4.1 and 4.2. Results show that multiplication factors change as a function of the NJOY version used. For example, the difference between the MCNP4C original library and the library generated with NJOY99.81 is 394 pcm in case 19; the difference is 815 pcm using YUMMY. Also, note that multiplication factors generated using YUMMY are mostly higher (and closer to unity) than the ones generated by the MCNP4C original library. Additionally, Table 4.3 presents the results predicted at temperatures 373.15, 423.15, 473.15, 523.15, and 587 K using YUMMY. The original benchmark cases are not at these temperatures; however, these calculations were performed to test the multi-temperature data in YUMMY.

The new ACE library and MCNP4C original library were also used to calculate multiplication factors for MCNP models provided by YMP staff. The first two cases are commercial reactor critical models for the Crystal River Unit 3, Cycle 5, which is a Babcock and Wilcox PWR design. The reactor was modeled in eighth core symmetry for effective full power days state-points of 0.0 and 388.5. In addition, YMP provided MCNP models for PWR and BWR waste package configurations loaded with assemblies at 3.5 weight percent initial enrichment and 30 giga-watt-day/metric-ton-uranium burnup. These models were also used in MCNP4C with the MCNP4C original library and YUMMY. Table 4.4 gives the results for these models. The statistical uncertainties in the multiplication factors are less than 0.06% for all calculations. The MCNP4C original library and the new library have differences of less than 420 pcm for these models. Similar to the LEU-COMP-THERM-003 problem, the discrepancies are attributed to the differences in the NJOY versions and NJOY options used in generating the cross-section libraries.

**Table 4.1. MCNP4C original library and new library results at 294 K for LEU-COMP-THERM-003**

| | Multiplication factor ($k_{eff}$) | | |
|---|---|---|---|
| Case number | MCNP4C original library | YUMMY | New library generated from NJOY 99.81 |
| 1 | 0.98617 ± 0.00196 | 0.99246 ± 0.00185 | 0.98750 ± 0.00171 |
| 2 | 0.98530 ± 0.00171 | 0.98715 ± 0.00174 | 0.98987 ± 0.00181 |
| 3 | 0.98929 ± 0.00166 | 0.99211 ± 0.00158 | 0.99000 ± 0.00160 |
| 4 | 0.98458 ± 0.00174 | 0.98503 ± 0.00163 | 0.98975 ± 0.00178 |
| 5 | 0.98742 ± 0.00176 | 0.99020 ± 0.00171 | 0.98831 ± 0.00176 |
| 6 | 0.98415 ± 0.00154 | 0.98804 ± 0.00176 | 0.98802 ± 0.00166 |
| 7 | 0.98597 ± 0.00185 | 0.98964 ± 0.00160 | 0.98683 ± 0.00162 |
| 8 | 0.98778 ± 0.00185 | 0.98630 ± 0.00181 | 0.98869 ± 0.00151 |
| 9 | 0.97953 ± 0.00163 | 0.98322 ± 0.00078 | 0.98425 ± 0.00076 |
| 10 | 0.97949 ± 0.00174 | 0.98380 ± 0.00171 | 0.98312 ± 0.00167 |
| 11 | 0.98360 ± 0.00169 | 0.98660 ± 0.00183 | 0.98364 ± 0.00155 |
| 12 | 0.98118 ± 0.00165 | 0.98292 ± 0.00167 | 0.98121 ± 0.00169 |
| 13 | 0.98570 ± 0.00162 | 0.98438 ± 0.00170 | 0.98585 ± 0.00188 |
| 14 | 0.98042 ± 0.00164 | 0.98548 ± 0.00153 | 0.98886 ± 0.00160 |
| 15 | 0.98496 ± 0.00171 | 0.98455 ± 0.00183 | 0.98881 ± 0.00164 |
| 16 | 0.98328 ± 0.00176 | 0.98457 ± 0.00169 | 0.98786 ± 0.00156 |
| 17 | 0.98232 ± 0.00174 | 0.9815 ± 0.001690 | 0.98488 ± 0.00149 |
| 18 | 0.98160 ± 0.00172 | 0.98319 ± 0.00172 | 0.98471 ± 0.00161 |
| 19 | 0.98105 ± 0.00168 | 0.98920 ± 0.00181 | 0.98499 ± 0.00171 |
| 20 | 0.98390 ± 0.00139 | 0.98485 ± 0.00151 | 0.98536 ± 0.00177 |
| 21 | 0.98094 ± 0.00157 | 0.98412 ± 0.00175 | 0.98434 ± 0.00183 |
| 22 | 0.99495 ± 0.00162 | 0.99130 ± 0.00171 | 0.99436 ± 0.00160 |
| 23 | 0.99295 ± 0.00166 | 0.99415 ± 0.00180 | 0.99614 ±0.00154 |

**Table 4.2. Effect of using NJOY99.90 and NJOY99.81 on LEU-COMP-THERM-003 results**

| | $k_{eff,\ MCNP\ original\ library}$ - $k_{eff,\ new\ library}$ | |
|---|---|---|
| Case number | New library generated by NJOY99.90 (YUMMY) | New library generated by NJOY99.81 |
| 1 | 629 | 133 |
| 2 | 185 | 457 |
| 3 | 282 | 71 |
| 4 | 45 | 517 |
| 5 | 278 | 89 |
| 6 | 389 | 387 |
| 7 | 367 | 86 |
| 8 | −148 | 91 |
| 9 | 369 | 472 |
| 10 | 431 | 363 |
| 11 | 300 | 4 |
| 12 | 174 | 3 |
| 13 | −132 | 15 |
| 14 | 506 | 844 |
| 15 | −41 | 385 |
| 16 | 129 | 458 |
| 17 | −82 | 256 |
| 18 | 159 | 311 |
| 19 | 815 | 394 |
| 20 | 95 | 146 |
| 21 | 318 | 340 |
| 22 | −365 | −59 |
| 23 | 120 | 319 |

**Table 4.3. The new library results for temperatures at 373.15 K, 423.15 K, 473.15 K, 523.15 K, 587 K for LEU-COMP-THERM-003**

| | Multiplicaton factors as a function of temperature | | | | |
|---|---|---|---|---|---|
| Case number | 373.15 K | 423.15 K | 473.15 K | 523.15 K | 587 K |
| 1 | 0.98643 ± 0.00173 | 0.98556 ± 0.00165 | 0.98111 ± 0.00167 | 0.98342 ± 0.00172 | 0.98150 ± 0.00186 |
| 2 | 0.98424 ± 0.00153 | 0.98787 ± 0.00179 | 0.98341 ± 0.00169 | 0.98289 ± 0.00201 | 0.98180 ± 0.00162 |
| 3 | 0.98388 ± 0.00178 | 0.98599 ± 0.00179 | 0.98466 ± 0.00163 | 0.98191 ± 0.00169 | 0.98157 ± 0.00181 |
| 4 | 0.98939 ± 0.00173 | 0.98818 ± 0.00193 | 0.98275 ± 0.00173 | 0.98517 ± 0.00173 | 0.98382 ± 0.00178 |
| 5 | 0.99097 ± 0.00186 | 0.98827 ± 0.00174 | 0.98669 ± 0.00182 | 0.98219 ± 0.00159 | 0.98241 ± 0.00199 |
| 6 | 0.98742 ± 0.00168 | 0.98370 ± 0.00178 | 0.98126 ± 0.00164 | 0.98218 ± 0.00162 | 0.98402 ± 0.00175 |
| 7 | 0.98620 ± 0.00179 | 0.98634 ± 0.00165 | 0.98777 ± 0.00182 | 0.98375 ± 0.00185 | 0.98296 ± 0.00155 |
| 8 | 0.98911 ± 0.00151 | 0.98570 ± 0.00173 | 0.98793 ± 0.00185 | 0.98366 ± 0.00179 | 0.98746 ± 0.00139 |
| 9 | 0.98272 ± 0.00166 | 0.98301 ± 0.00160 | 0.97978 ± 0.00184 | 0.97903 ± 0.00186 | 0.97836 ± 0.00168 |
| 10 | 0.97959 ± 0.00165 | 0.97922 ± 0.00174 | 0.97999 ± 0.00149 | 0.97891 ± 0.00166 | 0.97796 ± 0.00172 |
| 11 | 0.98482 ± 0.00153 | 0.98243 ± 0.00175 | 0.97961± 0.00168 | 0.98059 ± 0.00166 | 0.98078 ± 0.00171 |
| 12 | 0.98215 ± 0.00150 | 0.98077 ± 0.00174 | 0.98025 ± 0.00181 | 0.97629 ± 0.00183 | 0.97692 ± 0.00139 |
| 13 | 0.98568 ± 0.00166 | 0.98537 ± 0.00169 | 0.98399 ± 0.00162 | 0.98181 ± 0.00170 | 0.97917 ± 0.00162 |
| 14 | 0.98446 ± 0.00146 | 0.98095 ± 0.00161 | 0.98181 ± 0.00161 | 0.98134 ± 0.00174 | 0.97756 ± 0.00171 |
| 15 | 0.98159 ± 0.00176 | 0.98309 ± 0.00154 | 0.98304 ± 0.00173 | 0.98003 ± 0.00188 | 0.97906 ± 0.00160 |
| 16 | 0.98478 ± 0.00169 | 0.98500 ± 0.00170 | 0.98460 ± 0.00186 | 0.98156 ± 0.00182 | 0.97968 ± 0.00172 |
| 17 | 0.98216 ± 0.00173 | 0.97935 ± 0.00160 | 0.97952 ± 0.00185 | 0.98310 ± 0.00169 | 0.98228 ± 0.00177 |
| 18 | 0.98630 ± 0.00168 | 0.97900 ± 0.00180 | 0.98127 ± 0.00152 | 0.97873 ± 0.00177 | 0.97836 ± 0.00166 |
| 19 | 0.98172 ± 0.00175 | 0.98512 ± 0.00167 | 0.98218 ± 0.00175 | 0.98121 ± 0.00191 | 0.97887 ± 0.00176 |
| 20 | 0.98556 ± 0.00171 | 0.98298 ± 0.00201 | 0.98545 ± 0.00169 | 0.98116 ± 0.00195 | 0.97973 ± 0.00166 |
| 21 | 0.98555 ± 0.00164 | 0.98478 ± 0.00158 | 0.98055 ± 0.00156 | 0.97886 ± 0.00155 | 0.97577 ± 0.00182 |
| 22 | 0.99092 ± 0.00167 | 0.99170 ± 0.00172 | 0.98521 ± 0.00188 | 0.98901 ± 0.00171 | 0.98519 ± 0.00158 |
| 23 | 0.99055 ± 0.00160 | 0.98885 ± 0.00174 | 0.98812 ± 0.00169 | 0.99143 ± 0.00160 | 0.99084 ± 0.00161 |

**Table 4.4. MCNP4C original and new library comparisons**

| Cases | Multiplication factors | |
|---|---|---|
| | MCNP4C original library | YUMMY |
| PWR_1[a] | 0.99462 ± 0.00046 | 0.99882 ± 0.00044 |
| PWR_2[b] | 0.99712 ± 0.00044 | 1.00098 ± 0.00042 |
| PWR_WP[c] | 0.91646 ± 0.00063 | 0.91958 ± 0.00056 |
| BWR_WP[d] | 0.72805 ± 0.00045 | 0.73073 ± 0.00045 |

[a]Babcock and Wilcox (B&W) PWR reactor, effective full power day (EFPD) state-point = 0.0
[b]B&W PWR reactor, EFPD state-point = 388.5
[c]PWR waste package
[d]BWR waste package

## 5. SUMMARY

Continuous-energy ACE-format cross-sections were generated for 134 ENDF/B-V and ENDF/B-VI nuclides at seven temperatures (i.e., 0, 294, 373.15, 423.15, 473.15, 523.15 and 587 K) using the NJOY99.90 cross-section processing system. In an effort to test the point-wise data, resonance-integral calculations were performed for the total, elastic scattering, capture, and fission reactions, as a function of temperature. For verification purposes, continuous-energy cross-sections for the 134 nuclides were also generated with the AMPX-2000 code system. The same resonance integral calculations were performed with the AMPX-generated data and compared with the NJOY-based resonance integrals. The AMPX and NJOY results are in good agreement (within 1%) for the majority of the nuclides. Eleven of the nuclides have differences of more than 1%. Discrepancies are due to different processing methodologies in AMPX and NJOY.

The new cross-section library, YUMMY, was used in criticality benchmark cases for a PWR (commercial reactor critical) design at two different state-points, and for PWR and BWR waste package models in MCNP4C. Also, results obtained with the new library were compared with those predicted using the MCNP4C original library at 294 K. In general, results are in good agreement with the MCNP4C original library calculations, and discrepancies are attributed to different NJOY versions and options in generating the libraries. It should also be noted that YUMMY results show an improvement (the multiplication factor is closer to unity) for the criticality benchmark cases as well as the critical PWR designs. Based on the verification studies, the ACE-format cross-section data are acceptable for radiation transport calculations.

The new point-wise cross-section library YUMMY is provided in ASCII and big-endian binary ACE formats. Further work is ongoing to study temperature-based perturbation effects.

## 6. REFERENCES

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## Appendix A.

## ISOTOPES AND THEIR EVALUATIONS

| Symbol | MCNP ID | Evaluation Source Requested by YMP | Evaluation Source Used | Comments |
|---|---|---|---|---|
| h1 | 1001.50 | b-v.0[a] | b-v.0 | ENDF/B-V Release 0 |
| h3 | 1003.50 | b-v.0 | b-v.0 | |
| he4 | 2004.50 | b-v.0 | b-v.0 | |
| li6 | 3006.50 | b-v.0 | b-v.0 | |
| li7 | 3007.55 | b-v.2 | b-v.2 | ENDF/B-V Release 2 |
| be9 | 4009.50 | b-v.0 | b-v.0 | |
| B10 | 5010.50 | b-v.0 | b-v.0 | |
| b11 | 5011.56 | t2[b] | b-vi.0 | Replaced t2 with b-vi.0 |
| c | 6000.50 | b-v.0 | b-v.0 | |
| n14 | 7014.50 | b-v.0 | b-v.0 | |
| o16 | 8016.50 | b-v.0 | b-v.0 | |
| f19 | 9019.50 | b-v.0 | b-v.0 | |
| na23 | 11023.50 | b-v.0 | b-v.0 | |
| mg | 12000.50 | b-v.0 | b-v.0 | |
| al27 | 13027.50 | b-v.0 | b-v.0 | |
| si | 14000.50 | b-v.0 | b-v.0 | |
| p31 | 15031.50 | b-v.0 | b-v.0 | |
| s32 | 16032.50 | b-v.0 | b-v.0 | |
| cl | 17000.50 | b-v.0 | b-v.0 | |
| k | 19000.50 | b-v.0 | b-v.0 | |
| ca | 20000.50 | b-v.0 | b-v.0 | |
| ti | 22000.50 | b-v.0 | b-v.0 | |
| v | 23000.50 | b-v.0 | b-v.0 | |
| cr | 24000.50 | b-v.0 | b-v.0 | |
| cr50 | 24050.60 | b-vi.1 | b-vi.1 | ENDF/B-VI Release 1 |
| cr52 | 24052.60 | b-vi.1 | b-vi.1 | |
| cr53 | 24053.60 | b-vi.1 | b-vi.1 | |
| cr54 | 24054.60 | b-vi.1 | b-vi.1 | |
| mn55 | 25055.50 | b-v.0 | b-v.0 | |
| fe | 26000.55 | t2 | b-v.0 | Replaced t2 with b-v.0 |
| fe54 | 26054.60 | b-vi.1 | b-vi.1 | |
| fe56 | 26056.60 | b-vi.1 | b-vi.1 | |
| fe57 | 26057.60 | b-vi.1 | b-vi.1 | |
| fe58 | 26058.60 | b-vi.1 | b-vi.1 | |
| co59 | 27059.50 | b-v.0 | b-v.0 | |
| ni | 28000.50 | b-v.0 | b-v.0 | |
| ni58 | 28058.60 | b-vi.1 | b-vi.1 | |
| ni60 | 28060.60 | b-vi.1 | b-vi.1 | |
| ni61 | 28061.60 | b-vi.1 | b-vi.1 | |
| ni62 | 28062.60 | b-vi.1 | b-vi.1 | |
| ni64 | 28064.60 | b-vi.1 | b-vi.1 | |

## Appendix A – cont.

| Symbol | MCNP ID | Evaluation Source Requested by YMP | Evaluation Source Used | Comments |
|---|---|---|---|---|
| cu | 29000.50 | b-v.0 | b-v.0 | |
| cu63 | 29063.60 | b-vi.2 | b-vi.2 | ENDF/B-VI Release 2 |
| cu65 | 29065.60 | b-vi.2 | b-vi.2 | |
| as75 | 33075.35 | b-v.0 | b-v.0 | |
| kr80 | 36080.50 | b-v.0 | b-v.0 | |
| kr82 | 36082.50 | b-v.0 | b-v.0 | |
| kr83 | 36083.50 | b-v.0 | b-v.0 | |
| kr84 | 36084.50 | b-v.0 | b-v.0 | |
| kr86 | 36086.50 | b-v.0 | b-v.0 | |
| y89 | 39089.50 | b-v.0 | b-v.0 | |
| zr | 40000.56 | xtm.b-v[c] | - | |
| zr | 40000.60 | b-vi.1 | b-vi.1 | |
| zr93 | 40093.50 | b-v.0 | b-v.0 | |
| nb93 | 41093.50 | b-v.0 | b-v.0 | |
| mo | 42000.50 | b-v.0 | b-v.0 | |
| mo95 | 42095.50 | b-v.0 | b-v.0 | |
| tc99 | 43099.50 | b-v.0 | b-v.0 | |
| ru101 | 44101.50 | b-v.0 | b-v.0 | |
| ru103 | 44103.50 | b-v.0 | b-v.0 | |
| rh103 | 45103.50 | b-v.0 | b-v.0 | |
| rh105 | 45105.50 | b-v.0 | b-v.0 | |
| pd105 | 46105.50 | b-v.0 | b-v.0 | |
| pd108 | 46108.50 | b-v.0 | b-v.0 | |
| ag107 | 47107.60 | b-vi.0 | b-vi.0 | |
| ag109 | 47109.60 | b-vi.0 | b-vi.0 | |
| cd | 48000.50 | b-v.0 | b-v.0 | |
| in | 49000.60 | b-vi.0 | b-vi.0 | |
| sn | 50000.35 | llnl[d] | - | Could not find replacement for llnl |
| xe131 | 54131.50 | b-v.0 | b-v.0 | |
| xe134 | 54134.35 | llnl | b-vi.0 | Replaced llnl with b-vi.0 |
| xe135 | 54135.50 | b-v.0 | b-v.0 | |
| cs133 | 55133.50 | b-v.0 | b-v.0 | |
| cs135 | 55135.50 | b-v.0 | b-v.0 | |
| ba138 | 56138.50 | b-v.0 | b-v.0 | |
| pr141 | 59141.50 | b-v.0 | b-v.0 | |
| nd143 | 60143.50 | b-v.0 | b-v.0 | |
| nd145 | 60145.50 | b-v.0 | b-v.0 | |
| nd147 | 60147.50 | b-v.0 | b-v.0 | |
| nd148 | 60148.50 | b-v.0 | b-v.0 | |
| pm147 | 61147.50 | b-v.0 | b-v.0 | |
| pm148 | 61148.50 | b-v.0 | b-v.0 | |
| pm149 | 61149.50 | b-v.0 | b-v.0 | |
| sm147 | 62147.50 | b-v.0 | b-v.0 | |

## Appendix A – cont.

| Symbol | MCNP ID | Evaluation Source Requested by YMP | Evaluation Source Used | Comments |
|---|---|---|---|---|
| sm149 | 62149.50 | b-v.0 | b-v.0 | |
| sm150 | 62150.50 | b-v.0 | b-v.0 | |
| sm151 | 62151.50 | b-v.0 | b-v.0 | |
| sm152 | 62152.50 | b-v.0 | b-v.0 | |
| eu151 | 63151.55 | t2 | b-vi.0 | Replaced t2 with b-v.0 |
| eu152 | 63152.50 | b-v.0 | b-v.0 | |
| eu153 | 63153.55 | t2 | b-vi.7 | Replaced t2 with ENDF/B-VI Release 7 |
| eu154 | 63154.50 | b-v.0 | b-v.0 | |
| eu155 | 63155.50 | b-v.0 | b-v.0 | |
| gd152 | 64152.50 | b-v.0 | b-v.0 | |
| gd154 | 64154.50 | b-v.0 | b-v.0 | |
| gd155 | 64155.50 | b-v.0 | b-v.0 | |
| gd156 | 64156.50 | b-v.0 | b-v.0 | |
| gd157 | 64157.50 | b-v.0 | b-v.0 | |
| gd158 | 64158.50 | b-v.0 | b-v.0 | |
| gd160 | 64160.50 | b-v.0 | b-v.0 | |
| ho165 | 67165.55 | t2 | b-vi.5 | Replaced t2 with ENDF/B-VI Release 5 |
| hf | 72000.50 | b-v.0 | b-v.0 | |
| ta181 | 73181.50 | b-v.0 | b-v.0 | |
| ta182 | 73182.60 | b-vi.0 | b-vi.0 | |
| w182 | 74182.55 | b-v.2 | b-v.2 | |
| w183 | 74183.55 | b-v.2 | b-v.2 | |
| w184 | 74184.55 | b-v.2 | b-v.2 | |
| w | 74000.55 | b-v.2 | b-v.2 | |
| w186 | 74186.55 | b-v.2 | b-v.2 | |
| pb | 82000.50 | b-v.0 | b-v.0 | |
| th232 | 90232.50 | b-v.0 | b-v.0 | |
| pa233 | 91233.50 | b-v.0 | b-v.0 | |
| u233 | 92233.50 | b-v.0 | b-v.0 | |
| u234 | 92234.50 | b-v.0 | b-v.0 | |
| u235 | 92235.50 | b-v.0 | b-v.0 | |
| u236 | 92236.50 | b-v.0 | b-v.0 | |
| u237 | 92237.50 | b-v.0 | b-v.0 | |
| u238 | 92238.50 | b-v.0 | b-v.0 | |
| np235 | 93235.35 | llnl | - | Could not find replacement for llnl |
| np236 | 93236.35 | llnl | - | Could not find replacement for llnl |
| np237 | 93237.50 | b-v.0 | b-v.0 | |
| np238 | 93238.35 | llnl | b-vi.2 | Replaced llnl with b-vi.2 |
| pu237 | 94237.35 | llnl | b-vi.0 | Replaced llnl with b-vi.0 |
| pu238 | 94238.50 | b-v.0 | b-v.0 | |
| pu239 | 94239.55 | b-v.2 | b-v.2 | |
| pu240 | 94240.50 | b-v.0 | b-v.0 | |
| pu241 | 94241.50 | b-v.0 | b-v.0 | |
| pu242 | 94242.50 | b-v.0 | b-v.0 | |

## Appendix A – cont.

| Symbol | MCNP ID | Evaluation Source Requested by YMP | Evaluation Source Used | Comments |
|---|---|---|---|---|
| am241 | 95241.50 | b-v.0 | b-v.0 | |
| am242m | 95242.50 | b-v.0 | b-v.0 | |
| am243 | 95243.50 | b-v.0 | b-v.0 | |
| cm242 | 96242.50 | b-v.0 | b-v.0 | |
| cm243 | 96243.35 | llnl | b-vi.7 | Replaced llnl with ENDF/B-VI Release 7 |
| cm244 | 96244.50 | b-v.0 | b-v.0 | |
| cm245 | 96245.35 | llnl | b-vi.7 | Replaced llnl with b-vi.7 |
| cm246 | 96246.35 | llnl | b-vi.7 | Replaced llnl with b-vi.7 |
| cm247 | 96247.35 | llnl | b-vi.2 | Replaced llnl with b-vi.2 |
| cm248 | 96248.60 | b-vi.0 | b-vi.0 | |

[a]ENDF/B evaluation denoted with b-{version number}.{release number}. For example, b-v.0 refers to ENDF/B-V Release 0
[b]Internal LANL Group T2 evaluation
[c]Combination evaluation; internal LANL and ENDF/B-V
[d]Internal LLNL evaluation

## Appendix B.

## SAMPLE NJOY INPUTS

In this section, the execution sequences to process NJOY inputs for two isotopes are provided: $^{1}$H (unresolved data processing is not performed) and $^{238}$U (unresolved data processing is performed). The input decks were prepared with the execution sequence approach that is used in AMPX. The lines following "= shell" give a list of UNIX commands and those following "=njoy99" give the NJOY input decks.

### B.1. Point-wise Cross-Section Generation for $^{1}$H

```
=shell
ln -fs /projects/endf/endfv/t511 tape21
ln -fs /home/aa5/njoy99/njoy99/DEC_ver90/xnjoy njoy99
end
=njoy99
 reconr
  21 22
  'pendf tape for endfb-v.0  h1     MAT: 1301 '/
  1301 3 0/
  0.001 0/
  'h1    MAT 1301 Processed at ORNL  03/15/04'/
  'processed by the njoy system'/
  'm.e. dunn, 03/15/04   '/
  0/
 broadr
  21 22 23
  1301 6 0 0.0/
  0.001/
  294.00  373.15  423.15  473.15  523.15  587.00
  0/
 thermr
  0 23 24
  0 1301 16 6 1 0 1 221 1
  294.00  373.15  423.15  473.15  523.15  587.00
  0.001 5.0435
 stop
end
=shell
cat output > njoy.output
end
=njoy99
 acer
  21 22  0 25 26/
  1 1 1 .80/
  'endfb-v.0  h1     t=    0.00 processed at ORNL for YMP  03/15/04'/
  1301    0.00/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
```

```
cp tape25 /home/aa5/ymp/njoy/modules/acer/h1_0.00k
cp tape26 /home/aa5/ymp/njoy/mcnp.directory/h1_0.00k
end
=njoy99
 acer
  21 24  0 27 28/
  1 1 1 .81/
  'endfb-v.0  h1     t=  294.00 processed at ORNL for YMP  03/15/04'/
  1301  294.00/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape27 /home/aa5/ymp/njoy/modules/acer/h1_294.00k
cp tape28 /home/aa5/ymp/njoy/mcnp.directory/h1_294.00k
end
=njoy99
 acer
  21 24  0 29 30/
  1 1 1 .82/
  'endfb-v.0  h1     t=  373.15 processed at ORNL for YMP  03/15/04'/
  1301  373.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape29 /home/aa5/ymp/njoy/modules/acer/h1_373.15k
cp tape30 /home/aa5/ymp/njoy/mcnp.directory/h1_373.15k
end
=njoy99
 acer
  21 24  0 31 32/
  1 1 1 .83/
  'endfb-v.0  h1     t=  423.15 processed at ORNL for YMP  03/15/04'/
  1301  423.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape31 /home/aa5/ymp/njoy/modules/acer/h1_423.15k
cp tape32 /home/aa5/ymp/njoy/mcnp.directory/h1_423.15k
end
=njoy99
 acer
  21 24  0 33 34/
  1 1 1 .84/
  'endfb-v.0  h1     t=  473.15 processed at ORNL for YMP  03/15/04'/
```

```
  1301  473.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape33 /home/aa5/ymp/njoy/modules/acer/h1_473.15k
cp tape34 /home/aa5/ymp/njoy/mcnp.directory/h1_473.15k
end
=njoy99
 acer
  21 24  0 35 36/
  1 1 1 .85/
  'endfb-v.0  h1     t=  523.15 processed at ORNL for YMP  03/15/04'/
  1301  523.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape35 /home/aa5/ymp/njoy/modules/acer/h1_523.15k
cp tape36 /home/aa5/ymp/njoy/mcnp.directory/h1_523.15k
end
=njoy99
 acer
  21 24  0 37 38/
  1 1 1 .86/
  'endfb-v.0  h1     t=  587.00 processed at ORNL for YMP  03/15/04'/
  1301  587.00/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape37 /home/aa5/ymp/njoy/modules/acer/h1_587.00k
cp tape38 /home/aa5/ymp/njoy/mcnp.directory/h1_587.00k
cp njoy.output /home/aa5/ymp/njoy/inputs/h1.njoy.output
end
```

## B.2. Point-wise Cross-Section Generation for $^{238}$U

```
=shell
ln -fs /projects/endf/endfv/t516 tape21
ln -fs /home/aa5/njoy99/njoy99/DEC_ver90/xnjoy njoy99
end
=njoy99
 reconr
  21 22
```

```
  'pendf tape for endfb-v.0  u238   MAT: 1398 '/
  1398 3 0/
  0.001 0/
  'u238  MAT 1398 Processed at ORNL  03/15/04'/
  'processed by the njoy system'/
  'm.e. dunn, 03/15/04   '/
  0/
 broadr
  21 22 23
  1398 6 0 0.0/
  0.001/
  294.00  373.15  423.15  473.15  523.15  587.00
  0/
 unresr
  21 23 24
  1398 6 7 1
  294.00  373.15  423.15  473.15  523.15  587.00
  1.E+10  1.E+06  1.E+05  1.E+04  1.E+03  1.E+02  5.E+01
  0/
 purr
   21 24 25
  1398 6 7 20 32/
  294.00  373.15  423.15  473.15  523.15  587.00
  1.E+10  1.E+06  1.E+05  1.E+04  1.E+03  1.E+02  5.E+01
  0/
 thermr
  0 25 26
  0 1398 16 6 1 0 1 221 1
  294.00  373.15  423.15  473.15  523.15  587.00
  0.001 5.0435
 stop
end
=shell
cat output > njoy.output
end
=njoy99
 acer
  21 22  0 27 28/
  1 1 1 .80/
  'endfb-v.0  u238   t=    0.00 processed at ORNL for YMP  03/15/04'/
  1398    0.00/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape27 /home/aa5/ymp/njoy/modules/acer/u238_0.00k
cp tape28 /home/aa5/ymp/njoy/mcnp.directory/u238_0.00k
end
=njoy99
 acer
  21 26  0 29 30/
```

```
  1 1 1 .81/
  'endfb-v.0  u238   t=  294.00 processed at ORNL for YMP  03/15/04'/
  1398  294.00/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape29 /home/aa5/ymp/njoy/modules/acer/u238_294.00k
cp tape30 /home/aa5/ymp/njoy/mcnp.directory/u238_294.00k
end
=njoy99
 acer
  21 26  0 31 32/
  1 1 1 .82/
  'endfb-v.0  u238   t=  373.15 processed at ORNL for YMP  03/15/04'/
  1398  373.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape31 /home/aa5/ymp/njoy/modules/acer/u238_373.15k
cp tape32 /home/aa5/ymp/njoy/mcnp.directory/u238_373.15k
end
=njoy99
 acer
  21 26  0 33 34/
  1 1 1 .83/
  'endfb-v.0  u238   t=  423.15 processed at ORNL for YMP  03/15/04'/
  1398  423.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape33 /home/aa5/ymp/njoy/modules/acer/u238_423.15k
cp tape34 /home/aa5/ymp/njoy/mcnp.directory/u238_423.15k
end
=njoy99
 acer
  21 26  0 35 36/
  1 1 1 .84/
  'endfb-v.0  u238   t=  473.15 processed at ORNL for YMP  03/15/04'/
  1398  473.15/
  1/
  /
 stop
end
=shell
```

```
cat output >> njoy.output
cp tape35 /home/aa5/ymp/njoy/modules/acer/u238_473.15k
cp tape36 /home/aa5/ymp/njoy/mcnp.directory/u238_473.15k
end
=njoy99
 acer
  21 26  0 37 38/
  1 1 1 .85/
  'endfb-v.0  u238   t=  523.15 processed at ORNL for YMP  03/15/04'/
  1398  523.15/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape37 /home/aa5/ymp/njoy/modules/acer/u238_523.15k
cp tape38 /home/aa5/ymp/njoy/mcnp.directory/u238_523.15k
end
=njoy99
 acer
  21 26  0 39 40/
  1 1 1 .86/
  'endfb-v.0  u238   t=  587.00 processed at ORNL for YMP  03/15/04'/
  1398  587.00/
  1/
  /
 stop
end
=shell
cat output >> njoy.output
cp tape39 /home/aa5/ymp/njoy/modules/acer/u238_587.00k
cp tape40 /home/aa5/ymp/njoy/mcnp.directory/u238_587.00k
cp njoy.output /home/aa5/ymp/njoy/inputs/u238.njoy.output
end
```

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