

**YUMMY: THE YUCCA MOUNTAIN MCNP-  
LIBRARY**

**June 2004**



**YUMMY: THE YUCCA MOUNTAIN MCNP-LIBRARY**

**Prepared by:**

**F. A. Alpan  
and  
M. E. Dunn**

**April 2004**

**Prepared by  
OAK RIDGE NATIONAL LABORATORY  
managed by  
UT-BATTELLE, LLC  
for the  
U.S. DEPARTMENT OF ENERGY  
under contract DE-AC05-00OR22725**



## CONTENTS

	<u>Page</u>
LIST OF TABLES .....	vii
ACKNOWLEDGEMENTS .....	ix
ABSTRACT .....	xi
1. INTRODUCTION .....	1
2. THE TEMPERATURE-DEPENDENT LIBRARY DEVELOPMENT.....	1
3. TESTING .....	3
4. APPLICATION OF THE NEW LIBRARY .....	4
5. SUMMARY .....	8
6. REFERENCES .....	11
APPENDIX A. Isotopes and Their Evaluations .....	13
APPENDIX B. Sample NJOY Inputs .....	17



## LIST OF TABLES

<b>Table</b>		<b><u>Page</u></b>
4.1	MCNP4C Original Library and New Library Results at 294 K for LEU-COMP-THERM-003 .....	5
4.2	Effect of Using NJOY99.90 and NJOY99.81 on LEU-COMP-THERM-003 Result.....	6
4.3	The New Library Results for Temperatures at 373.15, 423.15, 473.15 523.15 587 K, for LEU-COMP-THERM-003 .....	7
4.4	MCNP4C Original and New Library Comparisons .....	8





## **ACKNOWLEDGEMENTS**

This work was sponsored by Bechtel-SAIC which manages and operates the Yucca Mountain Project for the Office of Civilian Radioactive Waste Management (OCRWM) of the U.S. Department of Energy.

The authors would like to acknowledge Dan Thomas as the manager responsible for this work, and both him and Abdelhalim Alsaed for technical support and guidance. We would also like to thank Joyce Echols for her help in the preparation of this manuscript.



## ABSTRACT

Point-wise 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 MCNP<sup>1</sup> for 138 nuclides, based on ENDF/B-V, ENDF/B-VI, Los Alamos National Laboratory (LANL) or Lawrence Livermore National Laboratory (LLNL) evaluations. Due to the unavailability of evaluations from LANL and LLNL, 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 4 of the isotopes and therefore, were not processed. As a result, cross sections for 134 isotopes were processed for 7 temperatures, including 0, 294, 373.15, 423.15, 473.15, 523.15, and 587 K, using NJOY99.90<sup>2</sup>. The new library is referred to as YUMMY (YUcca Mountain MCNP-library).

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<sup>3</sup> 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 point-wise, 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. One hundred twenty-two of the evaluations 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 evaluation 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 database 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 Zr evaluations developed at LANL was replaced with an ENDF/B-VI evaluation that was the same as that requested for the other Zr evaluation. Thus,

only one Zr evaluation was processed. As a result, a total of 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  $^1\text{H}$  and  $^{238}\text{U}$ . The input deck for  $^1\text{H}$  gives a sample NJOY processing procedure for an isotope that does not have unresolved data processing as opposed to  $^{238}\text{U}$  where unresolved data are processed. The modules used in NJOY for this work include: 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: (i) an ACE-format nuclear data table, and (ii) 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 of character information (e.g. nuclide identifier, atomic ratio, etc.), counters (e.g., length of the second block of data, number of energies, etc.) and pointers (e.g., location of energy table, location of cross sections, etc.). 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, the 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 forms a data library.

In this work, a total of 938 (134 nuclides at seven different temperatures) ASCII ACE-formatted files 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 name 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:

- (i) Nuclear data tables/cross-section libraries,
- (ii) A data directory file,

(iii) 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 forms a library exists.

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 due to their portability between different platforms. However, reading data from a sequential access ASCII file is more time-consuming compared to a direct access binary file. Additionally, a binary file is smaller in size compared to that in ASCII. 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 percent 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 percent 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 point-wise 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 percent 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 percent 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 the majority 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,  $^{109}\text{Ag}$ ,  $^{152}\text{Gd}$ ,  $^{154}\text{Gd}$ ,  $^{156}\text{Gd}$ ,  $^{160}\text{Gd}$ , Pb,  $^{232}\text{Th}$ ,  $^{234}\text{U}$ ,  $^{237}\text{Np}$ ,  $^{243}\text{Am}$ . 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<sup>4</sup>. 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 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 differences between 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 used in the benchmark cases. The differences in results caused by using NJOY version 81 and 90 is 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 MCNP4C original library and the library



generated with NJOY99.81 has a difference of 394pcm in case 19, which 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 (B&W) PWR design. The reactor was modeled in eighth core symmetry for Effective Full Power Days (EFPD) 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 (GWd/MTU) 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 uncertainty in the multiplication factors are less than 0.06% for all calculations. The MCNP4C original library and new library have differences 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**

Case number	Multiplication factor ( $k_{\text{eff}}$ )		
	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**

Case Number	$k_{\text{eff, MCNP original library}} - k_{\text{eff, new library}}$	
	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**

Case number	Multiplicaton factors as a function of temperature				
	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 <sup>a</sup>	0.99462 ± 0.00046	0.99882 ± 0.00044
PWR_2 <sup>b</sup>	0.99712 ± 0.00044	1.00098 ± 0.00042
PWR_WP <sup>c</sup>	0.91646 ± 0.00063	0.91958 ± 0.00056
BWR_WP <sup>d</sup>	0.72805 ± 0.00045	0.73073 ± 0.00045

<sup>a</sup>B&W PWR reactor, EFPD state-point = 0.0

<sup>b</sup>B&W PWR reactor, EFPD state-point = 388.5

<sup>c</sup>PWR waste package

<sup>d</sup>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 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 PWR and BWR waste package models in MCNP4C. Also, results obtained with the new library were compared to 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

1. "MCNP4C Monte Carlo N-Particle Transport Code System," CCC-700/MCNP4C, Los Alamos National Laboratory (April 2000).
2. R. E. MacFarlane, D. W. Muir, "NJOY99.0 Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B-VI Data," PSR 480/NJOY99.0, Los Alamos National Laboratory (March 2000).
3. M. E. Dunn, N. M. Greene, "AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications," Trans. Am. Nucl. Soc., 86, 118-119 (2002).
4. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03, CD, September 2003 Edition.





## Appendix A

### ISOTOPES AND THEIR EVALUATIONS

Symbol	MCNP ID	Evaluation Source Requested by YMP	Evaluation Source Used	Comments
h1	1001.50	b-v.0 <sup>a</sup>	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 <sup>b</sup>	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	xm.b-v <sup>c</sup>	-	
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 <sup>d</sup>	-	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	

<sup>a</sup>ENDF/B evaluation denoted with b-{version number}.{release number}. For example b-v.0 refers to ENDF/B-V Release 0

<sup>b</sup>Internal LANL Group T2 evaluation

<sup>c</sup>combination evaluation; internal LANL and ENDF/B-V

<sup>d</sup>Internal LLNL evaluation

## Appendix B

### SAMPLE NJOY INPUTS

In this section the execution sequence to process NJOY inputs for 2 isotopes are provided: H-1 (unresolved data processing is not performed) and U-238 (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 “=njoy99” give the NJOY input decks.

#### B.1. Point-wise Cross Section Generation for Hydrogen

```
=shell
ln -fs /projects/endl/endlv/t511 tape21
ln -fs /home/aa5/njoy99/njoy99/DEC_ver90/xnjoy njoy99
end
=njoy99
reconr
  21 22
  'pendf tape for endlb-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/
  'endlb-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
```

## Appendix B – cont.

```
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'/
```

## Appendix B – cont.

```
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 Uranium-238

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

## Appendix B – cont.

```
'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/
```



## Appendix B – cont.

```
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
```

## Appendix B – cont.

```
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
```

## **DISTRIBUTION**