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OAK RIDGE NATIONAL LABORATORY

LOCKHEED MARTIN

Testing of Multi-pole Formalism and POLIDENT Continuous Energy Cross-Section Data for Criticality Safety Applications

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LETTER REPORT

Computational Physics and Engineering Division

Contract Program or Project Title:	**Development and Application of Criticality Safety Software for Licensing Review**
Subject of Document:	**Testing of Multi-pole Formalism and POLIDENT Continuous Energy Cross-Section Data for Criticality Safety Applications**
Type of Document:	**Letter Report**
Authors:	**M. E. Dunn and N. M. Greene**
Date Published:	**May 1999**
Responsible NRC Individual and NRC Office or Division:	**C. W. Nilsen (301) 415-6209 U.S. Nuclear Regulatory Commission**

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CONTENTS

LIST OF TABLES

LIST OF FIGURES

ACKNOWLEDGMENTS

I. INTRODUCTION

The tasks associated with the "Development and Applicability of Criticality Safety Software for Licensing Review" are documented in the DOE Laboratory Project and Cost Proposal for NRC Work (JCN W6479).[1] Six tasks are documented which address the upgrade to the AMPX code system.[2] Specifically, Task 11 addresses the testing of the AMPX code system in preparation for future release of the system outside the Oak Ridge National Laboratory (ORNL). The AMPX upgrade is intended to facilitate independent[a] processing of Version 6 formats of the Evaluated Nuclear Data File (ENDF) using state-of-the-art procedures. Consequently, a comprehensive and alternative processing capability would be available to generate neutron cross-section data for criticality safety licensing applications. Task 6 of the cost proposal identifies various subtasks for the AMPX upgrade. In particular, a module (POLIDENT) will be developed to produce continuous energy or point cross sections from ENDF Files 2 and 3 data. In addition, the AMPX system will be modified to incorporate the multi-pole formalism option for the resolved resonance region (RRR). To date, a substantial amount of code development is complete with regard to POLIDENT and multi-pole processing. In an effort to establish the new capabilities of the AMPX code system, comprehensive testing of the new codes and procedures is necessary. Based on the reporting requirements for Task 11 of the cost proposal, this letter report documents the testing of the multi-pole formalism and POLIDENT point data for criticality safety applications.

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[a]Currently, NJOY[3] is the only production level code system that has the capability to process ENDF/B-VI cross-section evaluations.

II. MULTI-POLE PROCESSING

II.1 AMPX Upgrade

The multi-pole method was developed at Argonne National Laboratory (ANL) as a rigorous alternative for processing resolved resonance data that is expressed in the Reich-Moore formalism.[11]   The multi-pole method has several calculational efficiencies that make it an attractive processing method. In particular, the resonance-resonance interference effects are contained in the poles[a] thereby alleviating the need for a double summation over the resonances. Furthermore, the multi-pole cross-section calculation does not require the matrix inversion associated with the Reich-Moore formalism that accounts for interactions between the different reactions. In addition, the terms of the equations associated with the multi-pole method are linear combinations of terms that have the same form as observed in the Single Level Breit Wigner (SLBW) and Multi-Level Breit Wigner (MLBW) equations. Consequently, the cross sections can be Doppler broadened using efficient analytical expressions that do not require numerical integrations. In particular, the method for Doppler broadening is computationally similar to the approach of the widely used ψ and χ-routines; however, the approximations and inaccuracies associated with the ψ and χ-routines (e.g., neglecting motion of target nucleus) can be avoided.

Several procedures were developed to accommodate multi-pole parameters in AMPX. First, the WHOPPER code, which was developed at ANL to calculate the pole parameters from Reich-Moore data, was modified to remove several options not needed by the ORNL codes. In addition, WHOPPER was modified to interface efficiently with other ORNL codes. These modifications led to the development of two new codes: (1) INFA reads the ENDF/B file and stores the ENDF data in a format that is more amenable for processing Reich-Moore parameters, and (2) WHOPPOR reads the modified cross-section file from INFA and calculates the multi-pole parameters. Subsequently, the calculated parameters are stored by WHOPPOR in a new format designed for an AMPX master cross-section file. It should be noted that INFA and WHOPPOR have been combined into a single code named KRYSTAL. By combining the operations of INFA and WHOPPOR into a single code, the calculational procedures can be performed in a manner that is more suitable for the AMPX code system. The new code is named KRYSTAL in recognition that the stripped-down version of the WHOPPER code does not have all the capabilities of the original code.

The NITAWL and BONAMI codes are used in the SCALE system for resonance self-shielding calculations. NITAWL-II is the current SCALE module which generates resonance self-shielded cross sections in the resolved resonance region (RRR) using the Nordheim Integral Treatment. BONAMI generates resonance self-shielded cross sections in the unresolved resonance region. Based on the requirements for processing multi-pole data compared with the existing capabilities of NITAWL-II, a replacement module for NITAWL-II was developed and named NITAWL-III. In order to process the multi-pole data, a new method is needed to permit storage of the multi-pole parameters in an AMPX master library. The following sections discuss the required changes to the AMPX master library format as well as the development of NITAWL-III.

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[a]The use of the word "pole" in the text refers to multi-pole parameters.

II.1.1 New AMPX Resonance Parameter Formats

The multi-pole parameters consist of complex numbers for "energy," "scattering cross section," "capture cross section," and "fission cross section." Since the multi-pole terms are complex values, 8 parameters are required to represent a single pole. The mathematical operations for generating cross-section values typically require the difference of two numbers which could be very small (i.e., outside the limits of single-precision values). In order to calculate accurate cross-section values, the pole parameters must be stored and processed in a double-precision format.

The existing AMPX formats are in single precision, and there are between 50 and 100 codes that read master cross-section libraries in a single-precision format. Moreover, there are a couple of very important codes that convert the master libraries to a card-image format by reading the data in a single-precision format. Changing the AMPX master library to a double-precision format would require modifications to every code that processes an AMPX master library. The undesirable task of patching so many codes is not practical and could not be completed as part of the AMPX upgrade. Therefore, a new format must be developed that permits the specification of double-precision values in a single-precision format. Once developed, the new format can be used within the existing AMPX code system.

Resolved resonance parameters are stored in groups of 6-words per resonance, and the data directory for a nuclide tells how many of these 6-word groups are stored. A double-precision value can be adequately represented in single precision by separating the double-precision terms into two single-precision terms. Prior to use in an application, the two terms are summed to create a double-precision value. For example, the double-precision value of 1.2345678901234 can be stored as two single-precision words with values of 1.23456 and 0.00000789012, respectively. Single-precision 32-bit words can represent 6-digits on any platform, and using this procedure will provide a 12-digit "double-precision" value which is adequate for processing multi-pole parameters. With regard to processing multi-pole data, 8 parameters are required to represent each pole as noted previously. Using the pseudo-double precision scheme doubles the storage requirement to 16 words per pole.

Based on quality assurance needs coupled with a need to have the neutron width, Γ_n, available for determining an energy mesh for the cross-section calculation, the Reich-Moore parameters that were used to produce the multi-pole parameters should be included in the new format. An additional advantage is obtained by having the Reich-Moore parameters on a master library in case there is a need to process these parameters. Reich-Moore parameters consists of the resonance energy, a total width, a scattering width, a gamma width, and two fission width terms. As a result, each pole requires 6 additional words of data to be stored. (Note that the spin and angular momentum terms are stored elsewhere in the formats, such that they apply to a group of resonances and are not stored for individual resonances).

To accommodate the 6 words of Reich-Moore data, each Reich-Moore resonance requires two poles for a complete representation. In the new format, an arbitrary value of 20 words is allowed per pole. Moreover, 4 of the 6 words are stored with the data for the first pole, and the remaining 2 words are stored with the data for the second pole. A complete description of the resonance parameter format is provided in Appendix A.

II.1.2 NITAWL-III Development

NITAWL-II is written in a manner that is not amenable to the introduction of the multi-pole treatment. As noted previously, the multi-pole representation requires more parameters per pole than are used for Breit Wigner resonances. Furthermore, the multi-pole parameters must be represented in more precision than is possible using 32-bit single-precision arithmetic. As a result, the existing master library resonance parameter formats must be changed to accommodate the multi-pole parameters. Furthermore, in the Breit Wigner equations, the equations for n-gamma and fission cross sections have the same form. Using the similarity for the n-gamma and fission equations, NITAWL-II calculates an "absorption" cross section that is apportioned with one piece as the n-gamma cross section (after the point data are group-averaged), and the remaining piece as the fission cross section. The NITAWL-II calculation of the absorption cross section is not suitable for the multi-pole case because the fission cross section can have a different peak and shape than the n-gamma cross section. In addition, all of the Breit Wigner characteristics are directly coded into the group-averaging routines. In the multi-pole case, the n-gamma cross-section arrays must be carried independently from the fission cross-section arrays, thereby, requiring a re-write of the group-averaging routines.

The modifications to NITAWL were completed in a manner which removed some confusing variable names, eliminated many /common/ blocks, etc. As a result, a new code was developed that is easier to read and maintain.

II.1.3 Code to Compare NITAWL-II and NITAWL-III

Initially, the new NITAWL and its predecessor were compared by making visual examinations of the outputs from both codes. While this form of comparison permits the location of serious differences and inadvertent errors, the effort quickly reaches a point where the differences are not discernable by visual comparisons.   The Monte Carlo code KENO V.a was subsequently used to analyze various critical experiments using the NITAWL-III cross sections. Based on comparisons with KENO V.a calculations using NITAWL-II cross sections, the observed differences in the calculated k_{eff} values are practically within the Monte Carlo statistical deviations. However, for some cases, the differences in the calculated system multiplication warranted a close comparison between the NITAWL-II and NITAWL-III self-shielded cross sections. To facilitate these comparisons, a code was developed to compare two AMPX working libraries from the two versions of NITAWL. The new code performs a number-by-number comparison of the hundreds of numbers that are subsequently used in the transport calculation. The comparison code has the capability to report significant differences in the working libraries.

II.2 Testing

Processing multi-pole parameters required several modifications to the AMPX code system. The requisite modifications are discussed in Section II.1. Before the multi-pole parameters could be used for criticality safety applications, the resonance processing code NITAWL needed to be updated to calculate the cross sections using the multi-pole parameters. The latest version of the processing code is NITAWL-III.

Using the equation for the collision density, NITAWL-III calculates the neutron flux as a function of energy in a material region with a resonance absorber and a maximum of two admixed moderators. The multi-pole parameters are used to calculate the cross sections in the collision density equation for the problem of interest. Based on the collision density, the neutron flux is calculated and used to determine group averaged cross sections which are problem-dependent.

Before the multi-pole parameters can be used for criticality safety applications, the new codes and procedures must be tested using acceptable benchmark experiments. Previous validation efforts using the 199-group VITAMIN-B6 library in SCALE/CSAS25 have identified calculational problems for low-enriched thermal homogeneous systems with low H/U ratios (i.e., H/U < 8).[5] The 199-group library was generated from ENDF/B-VI data using the NJOY code system. The narrow resonance (NR) approximation with NJOY was used to prepare Bondarenko shielding factors over the entire energy range for all nuclides. Subsequently, the AMPX module SMILER was used to convert the NJOY library to an AMPX master library format, and the BONAMI module of SCALE was used for problelm-dependent processing. By virtue of the NR approximation, the collision density is assumed to be constant across the resonance, and there is complete flux recovery on the lower side (i.e., in energy) of the resonance. The NR approximation should only be used when the width of the resonance is narrow relative to the average scattering width. Low enriched uranium systems with low H/U values are strongly influenced by the ^{238}U capture cross-section resonances which are wide relative to the scattering width. Consequently, the NR approximation for these systems is inadequate because the approximation does not account for the significant amount of ^{238}U capture. As a result, the neutron flux on the lower energy side of the resonance is too high and the evaluated capture cross section is too low. Using the NR approximation for low enriched uranium systems with low H/U values could lead to higher calculated k_{eff} values which are incorrect.

As noted above, the poor results obtained with the 199-group library for uranium systems which are low enriched and low moderated can be directly attributed to the treatment of ^{238}U resonances. Thus, it was decided to test the use of multi-pole parameters in these low enriched uranium experiments. In an effort to test the use of multi-pole parameters, pole parameters were generated for ^{238}U. Subsequently, the full range Bondarenko shielding factors for ^{238}U in the 199-group library were removed and replaced with partial range shielding factors in the unresolved energy range. The multi-pole parameters were added to ^{238}U in the 199-group library.

77 critical experiments which are documented in Reference 5 were calculated in an effort to test NITAWL-III and the revised 199-group library for criticality safety applications. A brief description of each experiment is provided in Table II.1. Seven of the experiments in Table II.1 are low enriched uranium criticals with H/U ratios below 8. In particular, the results provided in Reference 5 (with the 199-group library) for Cases 29, 39, 40, 82, 83, 84 and 85 overestimate critical by 1– 4.5%.

Two objectives can be accomplished by calculating the series of 77 benchmark critical experiments. First, these calculations can be used to establish the capability of NITAWL-III for generating self-shielded cross sections for criticality safety applications. Second, the multi-pole formalism can be evaluated for the class of problems which are difficult to calculate using the NR approximation.

Calculations for the 77 critical experiments were performed using the CSAS25 sequence in SCALE 4.4[6] with NITAWL-II replaced with NITAWL-III. Problem-dependent resonance processing of the 199-group data used NITAWL-III for ^{238}U and BONAMI for all other nuclides. Furthermore, the calculations were performed on CA01, CA02, CA04 and CA29 IBM RS/6000 workstations in the Computational Physics and Engineering Division at ORNL. With regard to the first testing objective, calculated results are presented in Table II.2 for the 238 ENDF/B-V library using CSAS25 with NITAWL-II and NITAWL-III (i.e., Columns A and B, respectively). For the 238-group results, the calculated k_{eff} values obtained with NITAWL-III self-shielded cross sections are within two standard deviations of the results obtained with NITAWL-II. The good agreement between the calculated results in Columns A and B demonstrates that the capabilities of NITAWL-II

are maintained in the latest version of NITAWL. Furthermore, NITAWL-III can be used to generate self-shielded cross sections for criticality safety applications.

Calculated results are also provided in Column C of Table II.2 for the critical experiments using the unmodified (i.e., no multi-pole parameters) 199-group library.   It should be noted that 8 experiments could not be calculated using the VITAMIN-B6 library because the library does not have cross sections for [113]In, [115]In, [204]In, [79]Br and [81]Br. Therefore, the remaining 69 experiments are calculated using the 199-group library. The results obtained with the unmodified VITAMIN-B6 library are consistent with the results presented in Reference 5.   In general, the results obtained with the unmodified 199-group library are in good agreement with the results obtained with the 238-group library; however, the results obtained with the 199-group library for Cases 82 through 85 are 1 – 2.5% higher relative to the 238-group library. These differences are consistent with the results presented in Reference 5. With regard to Cases 29, 39 and 40, the unmodified 199-group library provides calculated k_{eff} values which are slightly higher than the 238-group results. These seven cases are low enriched uranium criticals with low H/U ratios. The higher calculated k_{eff} values for these seven experiments can be attributed to the NR resonance approximation for [238]U over the entire resonance region.

Using the revised 199-group library (i.e., multi-pole parameters for [238]U), calculated results are presented in Column D of Table II.2. For the low enriched homogeneous uranium criticals, the multi-pole parameters for [238]U lead to a significant improvement in the calculated multiplication factor for Cases 82 through 85. With the NR approximation, the mean calculated k_{eff} for Cases 82 through 85 is 1.0277, and the maximum k_{eff} is 1.0382 ± 0.0016. By using the multi-pole parameters and corresponding Nordheim Integral treatment for [238]U, the mean calculated system multiplication factor for these 4 experiments is 1.0124 with a maximum system multiplication factor of 1.0222 ± 0.0016. As a result, using the Nordheim Integral treatment to generate self-shielded cross sections for [238]U leads to a 1.5% decrease in system multiplication relative to the NR approximation. For Cases 29, 39 and 40, the inclusion of the multi-pole parameters for [238]U also leads to calculated results which are consistent with the calculated k_{eff} values obtained with the 238-group library.

Based on the results in Table II.2, NITAWL-III can be used to generate problem-dependent self-shielded cross sections for criticality safety applications. In addition, AMPX and NITAWL-III can be used to process multi-pole parameters based on ENDF/B-VI data. The multi-pole parameters can be used in the Nordheim Integral treatment to determine the problem-dependent neutron flux and subsequent self-shield cross sections for criticality safety applications.

Table II.1: Test Case Descriptions[5]

Case No.	Case Identifier	Enrichment (wt %)	Description	Lattice Water/Fuel Volume Ratio
			LWR-type UO$_2$ Fuel Pin Lattices	
1	p2438x05	2.35	No absorber plates	2.92
2	p2438x17	2.35	Boral absorber plates	2.92
3	p2438x28	2.35	Stainless steel absorber plates	2.92
4	p2615x14	4.31	Stainless steel absorber plates	3.88
5	p2615x23	4.31	Cadmium absorber plates	3.88
6	p2615x31	4.31	Boral absorber plates	3.88
7	p2827u2a	2.35	Uranium reflector	2.92
9	p2827non	2.35	No reflector	2.92
10	p2827u2b	4.31	Uranium reflector	3.88
12	p3314a	4.31	0.226 cm Boroflex absorber plates	1.6
13	p3314b	4.31	0.452 cm Boroflex absorber plates	1.6
14	p3602n2	2.35	Steel reflector, no absorber	2.92
15	p3602non	4.31	Steel reflector, no absorber	1.6
16	p3602s4	4.31	Steel reflector, borated steel absorber plates	1.6
17	p3602b4	4.31	Steel reflector, Boral absorber plates	1.6
18	p3602c4	4.31	Steel reflector, cadmium absorber plates	1.6
19	p3926u2a	2.35	Uranium reflector	1.6
21	p3926n2	2.35	No reflector	1.6
22	p3926u4a	4.31	Uranium reflector	1.6
24	p3926nob	4.31	No reflector	1.6
25	p4267a	4.31	No soluble boron	1.59
26	p4267b	4.31	2550 ppm soluble boron	1.59
27	p4267c	4.31	No soluble boron	1.09
28	p4267d	4.31	2550 ppm soluble boron	1.09
29	pnl194	4.31	Hexagonal lattice, narrow pitch	0.509
30	ft214r	4.31	Flux traps, no voids	1.6
31	ft214v	4.31	Flux traps with voids	1.6
32	baw1231a	4	Core I - 1152 ppm soluble boron	0.994
33	baw1231b	4	Core I - 3389 ppm soluble boron	0.994
34	baw1273m	2.46	Core XX - 1675 ppm soluble boron	0.999
35	baw1484a	2.46	Core IV - 84 B4C pins - 1 pitch between assemblies	1.84
36	baw1484b	2.46	Core IX - No B4C pins - 4 pitches between assemblies	1.84
37	baw1484c	2.46	Core XIII - 1.6 wt % Boral - 1 pitch between assemblies	1.84
38	baw1484d	2.46	Core XXI - 0.1 wt % Boral - 3 pitches between assemblies	1.84
39	baw1645t	2.46	Triangular pitch, pitch = pin O. D.	0.149
40	baw1645s	2.46	Square pitch, pitch = pin O. D.	0.383
41	bw1645so	2.46	Square pitch, pitch = 1.17*pin O. D.	1.014

8

Table II.1 (continued)

Case No.	Case Identifier	Enrichment (wt %)	Description	Lattice Water/Fuel Volume Ratio
42	bnw1810a	2.46 and 4.02	Core 12 - No Gd fuel rods	1.84 and 1.53
46	epru615b	2.35	0.615 in. pitch, 464 ppm soluble boron	1.196
47	epru75	2.35	0.750 in. pitch, 0 ppm soluble boron	2.408
48	epru75b	2.35	0.750 in. pitch, 568 ppm soluble boron	2.408
50	epru87b	2.35	0.870 in. pitch, 286 ppm soluble boron	3.687
51	saxu56	5.74	2 lattice pitches, SS clad, 0.56 in. pitch	1.933
52	saxu792	5.74	2 lattice pitches, SS clad, 0.792 in. pitch	5.067
54	w3269b	3.7	Ag-In-Cd (0.330 in. O.D.) Absorber rods, 0.435 in. pitch	2.9
56	ans33b2	4.75	Cruciform box, polyethylene powder absorbers	1.81
57	ans33bb2	4.75	Cruciform box, polyethylene ball absorbers	1.81
58	ans33bh2	4.75	Cruciform box only	1.81
59	ans33h2	4.75	No absorbers	1.81
			LWR-type Mixed-Oxide (UO_2-PuO_2) Fuel Pin Lattices	
60	epri70un	^{235}U: 0.72 ^{239}Pu: 90	0.700 in. pitch, 0 ppm soluble boron, 2 wt % PuO_2	1.195
61	epri70b	^{235}U: 0.72 ^{239}Pu: 90	0.700 in. pitch, 681ppm soluble boron, 2 wt % PuO_2	1.195
62	epri87un	^{235}U: 0.72 ^{239}Pu: 90	0.870 in. pitch, 0 ppm soluble boron	1.527
63	epri87b	^{235}U: 0.72 ^{239}Pu: 90	0.870 in. pitch, 1090 ppm soluble boron, 2 wt % PuO_2	1.527
64	epri99un	^{235}U: 0.72 ^{239}Pu: 90	0.990 in. pitch, 0 ppm soluble boron, 2 wt % PuO_2	3.641
65	epri99b	^{235}U: 0.72 ^{239}Pu: 90	0.990 in. pitch, 767 ppm soluble boron, 2 wt % PuO_2	3.641
66	saxton52	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.52 in. pitch, 6.6 wt % PuO_2	1.681
67	saxton56	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.56 in. pitch, 6.6 wt % PuO_2	2.165
68	saxtn56b	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.56 in. pitch, 337 ppm boron, 6.6 wt % PuO_2	2.165
69	saxtn735	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.735 in. pitch, 6.6 wt % PuO_2	4.699
70	saxtn792	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 0.792 in. pitch, 6.6 wt % PuO_2	5.673
71	saxtn104	^{235}U: 0.72 ^{239}Pu: 90	UO_2/PuO_2 square lattice, 1.04 in. pitch, 6.6 wt % PuO_2	10.754

Table II.1 (continued)

Case No.	Case Identifier	Enrichment (wt %)	Description	Lattice Water/Fuel Volume Ratio
			Fast Reactor (FFTF) Mixed-Oxide (UO_2-PuO_2) Fuel Pin Lattices	
73	p5803x21	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 0.968 cm pitch, 20 wt % PuO_2	3.49
74	p5803x32	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 1.935 cm pitch, 20 wt % PuO_2	18.13
75	p5803x43	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 1.242 cm pitch, 20 wt % PuO_2	6.65
76	p5803x67	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 0.761 cm pitch, 20 wt % PuO_2	1.62
77	p5803x68r	^{235}U: 0.72 ^{239}Pu: 86	FFTF rods, H_2O Moderated, 1.537 cm pitch, 20 wt % PuO_2	10.93
			Low-Enriched Homogeneous Uranium Criticals	
82	ydr14un2	2	Homogenized uranium in paraffin, unreflected	$H/^{235}U$: 293.9
83	ydr14pl2	2	Homogenized uranium in paraffin, plexiglas & paraffin reflectors	$H/^{235}U$: 406.3
84	ydr14pl3	3	Homogenized uranium in paraffin, plexiglas & paraffin reflectors	$H/^{235}U$: 133.4
85	ydr14un3	3	Homogenized uranium in paraffin, unreflected	$H/^{235}U$: 133.4
			High-Enriched Uranium Solutions	
86	or260901	93.2	UO_2F_2 solution sphere, no reflector	$H/^{235}U$: 1112
87	or260906	93.2	UO_2F_2 solution sphere, H_2O reflector	$H/^{235}U$: 1270
88	rfp2710u	93.2	$UO_2(NO_3)_2$ solution, 142.9 g U/l, cylinder, no reflector	
89	rfp2710r	93.2	$UO_2(NO_3)_2$ solution, 345.3 g U/l, cylinder, plexiglas reflector	
90	or2968s1	4.89	UO_2F_2 solution, 42.54 g ^{235}U/l, SS cylinder, no reflector	$H/^{235}U$: 524
91	or2968al	4.89	UO_2F_2 solution, 42.54 g ^{235}U/l, Al box, H_2O reflector	$H/^{235}U$: 524
92	or2968s2	4.89	UO_2F_2 solution, 24.22 g ^{235}U/l, SS cylinder, no reflector	$H/^{235}U$: 994

Table II.2: Calculated Results for Testing NITAWL-III and 199-Group VITAMIN-B6 Library with ^{238}U Multi-pole Data

Case No.	Case Designation	$k_{eff} \pm \sigma$				Δk			
		238-group (NITAWL-II Revised) (A)	238-group (NITAWL-III Revised) (B)	199g VITAMIN-B6 (BONAMI) (C)	199g VITAMIN-B6/^{238}U-Multi-pole Parameters (NITAWL-III Revised) (D)	(B-A)	(C-B)	(D-B)	(D-C)
1	p2438x05	0.9964 ± 0.0016	0.9938 ± 0.0016	0.9948 ± 0.0014	0.9930 ± 0.0015	-0.0026	0.0010	-0.0008	-0.0018
2	p2438x17	0.9958 ± 0.0011	0.9961 ± 0.0013	0.9923 ± 0.0012	0.9938 ± 0.0010	0.0003	-0.0038	-0.0023	0.0015
3	p2438x28	0.9959 ± 0.0017	0.9982 ± 0.0013	0.9931 ± 0.0016	0.9912 ± 0.0015	0.0023	-0.0051	-0.0070	-0.0019
4	p2615x14	0.9963 ± 0.0016	0.9963 ± 0.0016	0.9901 ± 0.0015	0.9916 ± 0.0015	0.0000	-0.0062	-0.0047	0.0015
5	p2615x23	0.9986 ± 0.0016	0.9979 ± 0.0016	0.9932 ± 0.0019	0.9916 ± 0.0015	-0.0007	-0.0047	-0.0063	-0.0016
6	p2615x31	1.0004 ± 0.0016	0.9980 ± 0.0018	0.9951 ± 0.0016	0.9944 ± 0.0018	-0.0024	-0.0029	-0.0036	-0.0007
7	p2827u2a	0.9980 ± 0.0015	0.9980 ± 0.0017	0.9967 ± 0.0016	0.9940 ± 0.0016	0.0000	-0.0013	-0.0040	-0.0027
9	p2827non	0.9922 ± 0.0016	0.9965 ± 0.0015	0.9916 ± 0.0014	0.9890 ± 0.0013	0.0043	-0.0049	-0.0075	-0.0026
10	p2827u2b	0.9961 ± 0.0017	0.9958 ± 0.0018	0.9976 ± 0.0017	0.9958 ± 0.0018	-0.0003	0.0018	0.0000	-0.0018
12	p3314a	1.0000 ± 0.0018	1.0018 ± 0.0017	0.9996 ± 0.0017	0.9950 ± 0.0016	0.0018	-0.0022	-0.0068	-0.0046
13	p3314b	0.9972 ± 0.0013	0.9981 ± 0.0013	0.9951 ± 0.0014	0.9966 ± 0.0014	0.0009	-0.0030	-0.0015	0.0015
14	p3602n2	0.9960 ± 0.0012	0.9976 ± 0.0014	0.9946 ± 0.0016	0.9940 ± 0.0014	0.0016	-0.0030	-0.0036	-0.0006
15	p3602non	0.9991 ± 0.0018	0.9995 ± 0.0017	0.9958 ± 0.0017	0.9953 ± 0.0018	0.0004	-0.0037	-0.0042	-0.0005
16	p3602s4	1.0000 ± 0.0019	0.9997 ± 0.0019	0.9937 ± 0.0016	0.9944 ± 0.0018	-0.0003	-0.0060	-0.0053	0.0007
17	p3602b4	0.9992 ± 0.0018	1.0020 ± 0.0020	0.9972 ± 0.0016	0.9948 ± 0.0017	0.0028	-0.0048	-0.0072	-0.0024
18	p3602c4	0.9973 ± 0.0013	0.9985 ± 0.0013	0.9934 ± 0.0013	0.9917 ± 0.0012	0.0012	-0.0051	-0.0068	-0.0017
19	p3926u2a	0.9953 ± 0.0017	0.9967 ± 0.0015	0.9913 ± 0.0018	0.9886 ± 0.0013	0.0014	-0.0054	-0.0081	-0.0027

Table II.2 (continued)

Case No.	Case Designation	k_eff ± σ				Δk			
		238-group (NITAWL-II Revised) (A)	238-group (NITAWL-III Revised) (B)	199g VITAMIN-B6 (BONAMI) (C)	199g VITAMIN-B6/^{238}U-Multi-pole Parameters (NITAWL-III Revised) (D)	(B-A)	(C-B)	(D-B)	(D-C)
21	p3926n2	0.9928 ± 0.0016	0.9924 ± 0.0016	0.9925 ± 0.0016	0.9880 ± 0.0017	-0.0004	0.0001	-0.0044	-0.0045
22	p3926u4a	0.9978 ± 0.0020	0.9965 ± 0.0019	0.9948 ± 0.0017	0.9946 ± 0.0018	-0.0013	-0.0017	-0.0019	-0.0002
24	p3926nob	0.9954 ± 0.0017	0.9968 ± 0.0018	0.9927 ± 0.0017	0.9908 ± 0.0016	0.0014	-0.0041	-0.0060	-0.0019
25	p4267a	0.9916 ± 0.0013	0.9950 ± 0.0011	0.9915 ± 0.0014	0.9917 ± 0.0011	0.0034	-0.0035	-0.0033	0.0002
26	p4267b	1.0007 ± 0.0016	0.9988 ± 0.0015	1.0000 ± 0.0014	0.9958 ± 0.0014	-0.0019	0.0012	-0.0030	-0.0042
27	p4267c	0.9951 ± 0.0012	0.9950 ± 0.0013	0.9933 ± 0.0012	0.9918 ± 0.0014	-0.0001	-0.0017	-0.0032	-0.0015
28	p4267d	0.9918 ± 0.0014	0.9903 ± 0.0016	0.9905 ± 0.0016	0.9914 ± 0.0013	-0.0015	0.0002	0.0011	0.0009
29	**pnl194**	**0.9954 ± 0.0015**	**0.9995 ± 0.0015**	**1.0051 ± 0.0015**	**0.9949 ± 0.0016**	**0.0041**	**0.0056**	**-0.0046**	**-0.0102**
30	ft214r	0.9953 ± 0.0018	0.9968 ± 0.0017	0.9941 ± 0.0017	0.9924 ± 0.0019	0.0015	-0.0027	-0.0044	-0.0017
31	ft214v	0.9921 ± 0.0012	0.9950 ± 0.0012	0.9930 ± 0.0011	0.9945 ± 0.0014	0.0029	-0.0020	-0.0005	0.0015
32	baw1231a	0.9922 ± 0.0011	0.9928 ± 0.0013	0.9936 ± 0.0010	0.9903 ± 0.0010	0.0006	0.0008	-0.0025	-0.0033
33	baw1231b	0.9926 ± 0.0009	0.9955 ± 0.0009	0.9967 ± 0.0012	0.9926 ± 0.0009	0.0029	0.0012	-0.0029	-0.0041
34	baw1273m	0.9948 ± 0.0012	0.9943 ± 0.0013	0.9960 ± 0.0013	0.9918 ± 0.0013	-0.0005	0.0017	-0.0025	-0.0042
35	baw1484a	0.9918 ± 0.0011	0.9926 ± 0.0014	0.9928 ± 0.0013	0.9919 ± 0.0012	0.0008	0.0002	-0.0007	-0.0009
36	baw1484b	0.9919 ± 0.0015	0.9940 ± 0.0014	0.9916 ± 0.0017	0.9834 ± 0.0016	0.0021	-0.0024	-0.0106	-0.0082
37	baw1484c	0.9964 ± 0.0016	0.9924 ± 0.0014	0.9942 ± 0.0014	0.9919 ± 0.0015	-0.0040	0.0018	-0.0005	-0.0023
38	baw1484d	0.9906 ± 0.0014	0.9908 ± 0.0015	0.9839 ± 0.0014	0.9889 ± 0.0015	0.0002	-0.0069	-0.0019	0.0050

12

Table II.2 (continued)

Case No.	Case Designation	$k_{eff} \pm \sigma$				Δk			
		238-group (NITAWL-II Revised) (A)	238-group (NITAWL-III Revised) (B)	199g VITAMIN-B6 (BONAMI) (C)	199g VITAMIN-B6/^{238}U-Multi-pole Parameters (NITAWL-III Revised) (D)	(B-A)	(C-B)	(D-B)	(D-C)
39	**baw1645t**	**0.9964 ± 0.0011**	**0.9968 ± 0.0011**	**1.0051 ± 0.0010**	**0.9954 ± 0.0011**	**0.0004**	**0.0083**	**-0.0014**	**-0.0097**
40	**baw1645s**	**0.9957 ± 0.0016**	**0.9928 ± 0.0013**	**1.0016 ± 0.0015**	**0.9936 ± 0.0018**	**-0.0029**	**0.0088**	**0.0008**	**-0.0080**
41	bw1645so	0.9938 ± 0.0013	0.9947 ± 0.0014	1.0003 ± 0.0014	0.9941 ± 0.0013	0.0009	0.0056	-0.0006	-0.0062
42	bnw1810a	0.9939 ± 0.0017	0.9942 ± 0.0011	0.9948 ± 0.0014	0.9981 ± 0.0016	0.0003	0.0006	0.0039	0.0033
46	epru615b	0.9956 ± 0.0018	0.9945 ± 0.0015	0.9984 ± 0.0017	0.9922 ± 0.0015	-0.0011	0.0039	-0.0023	-0.0062
47	epru75	0.9967 ± 0.0013	0.9949 ± 0.0012	0.9922 ± 0.0011	0.9905 ± 0.0012	-0.0018	-0.0027	-0.0044	-0.0017
48	epru75b	0.9970 ± 0.0011	0.9995 ± 0.0011	0.9965 ± 0.0010	0.9956 ± 0.0011	0.0025	-0.0030	-0.0039	-0.0009
50	epru87b	1.0003 ± 0.0014	0.9990 ± 0.0014	0.9953 ± 0.0012	0.9976 ± 0.0012	-0.0013	-0.0037	-0.0014	0.0023
51	saxu56	0.9951 ± 0.0020	0.9944 ± 0.0020	0.9873 ± 0.0016	0.9922 ± 0.0017	-0.0007	-0.0071	-0.0022	0.0049
52	saxu792	0.9958 ± 0.0015	0.9962 ± 0.0013	0.9941 ± 0.0014	0.9953 ± 0.0013	0.0004	-0.0021	-0.0009	0.0012
54	w3269b	0.9975 ± 0.0018	0.9975 ± 0.0015	a	a	0.0000	N/A	N/A	N/A
56	ans33b2	0.9966 ± 0.0015	0.9937 ± 0.0013	0.9950 ± 0.0013	0.9946 ± 0.0013	-0.0029	0.0013	0.0009	-0.0004
57	ans33bb2	1.0046 ± 0.0019	1.0069 ± 0.0015	1.0015 ± 0.0014	1.0034 ± 0.0012	0.0023	-0.0054	-0.0035	0.0019
58	ans33bh2	1.0093 ± 0.0013	1.0128 ± 0.0013	1.0058 ± 0.0012	1.0054 ± 0.0012	0.0035	-0.0070	-0.0074	-0.0004
59	ans33h2	0.9934 ± 0.0013	0.9929 ± 0.0012	0.9917 ± 0.0011	0.9910 ± 0.0012	-0.0005	-0.0012	-0.0019	-0.0007
60	epri70un	0.9966 ± 0.0018	0.9937 ± 0.0019	b	b	-0.0029	N/A	N/A	N/A
61	epri70b	0.9978 ± 0.0016	0.9991 ± 0.0016	b	b	0.0013	N/A	N/A	N/A

13

Table II.2 (continued)

Case No.	Case Designation	$k_{eff} \pm \sigma$				Δk			
		238-group (NITAWL-II Revised) (A)	238-group (NITAWL-III Revised) (B)	199g VITAMIN-B6 (BONAMI) (C)	199g VITAMIN-B6/238U-Multi-pole Parameters (NITAWL-III Revised) (D)	(B-A)	(C-B)	(D-B)	(D-C)
62	epri87un	0.9995 ± 0.0012	1.0021 ± 0.0011	b	b	0.0026	N/A	N/A	N/A
63	epri87b	1.0053 ± 0.0015	1.0051 ± 0.0018	b	b	-0.0002	N/A	N/A	N/A
64	epri99un	1.0041 ± 0.0015	1.0038 ± 0.0016	b	b	-0.0003	N/A	N/A	N/A
65	epri99b	1.0064 ± 0.0010	1.0065 ± 0.0010	b	b	0.0001	N/A	N/A	N/A
66	saxton52	0.9943 ± 0.0013	0.9930 ± 0.0013	0.9944 ± 0.0012	0.9924 ± 0.0013	-0.0013	0.0014	-0.0006	-0.0020
67	saxton56	0.9906 ± 0.0020	0.9961 ± 0.0020	0.9923 ± 0.0018	0.9937 ± 0.0017	0.0055	-0.0038	-0.0024	0.0014
68	saxtn56b	0.9925 ± 0.0019	0.9948 ± 0.0018	0.9929 ± 0.0019	0.9961 ± 0.0017	0.0023	-0.0019	0.0013	0.0032
69	saxtn735	1.0000 ± 0.0020	1.0005 ± 0.0021	0.9964 ± 0.0018	0.9958 ± 0.0018	0.0005	-0.0041	-0.0047	-0.0006
70	saxtn792	0.9995 ± 0.0020	1.0011 ± 0.0018	0.9951 ± 0.0021	0.9931 ± 0.0017	0.0016	-0.0060	-0.0080	-0.0020
71	saxtn104	1.0067 ± 0.0017	1.0007 ± 0.0017	0.9972 ± 0.0018	0.9990 ± 0.0016	-0.0060	-0.0035	-0.0017	0.0018
73	p5803x21	1.0008 ± 0.0013	1.0001 ± 0.0013	1.0002 ± 0.0012	1.0019 ± 0.0012	-0.0007	0.0001	0.0018	0.0017
74	p5803x32	1.0061 ± 0.0016	1.0044 ± 0.0017	1.0013 ± 0.0018	0.9998 ± 0.0018	-0.0017	-0.0031	-0.0046	-0.0015
75	p5803x43	1.0025 ± 0.0015	1.0004 ± 0.0011	0.9990 ± 0.0013	1.0003 ± 0.0012	-0.0021	-0.0014	-0.0001	0.0013
76	p5803x67	0.9991 ± 0.0010	0.9977 ± 0.0012	0.9960 ± 0.0011	0.9997 ± 0.0013	-0.0014	-0.0017	0.0020	0.0037
77	p5803x68r	1.0043 ± 0.0017	1.0042 ± 0.0017	0.9969 ± 0.0016	1.0011 ± 0.0017	-0.0001	-0.0073	-0.0031	0.0042
82	**ydr14un2**	**1.0038 ± 0.0016**	**1.0000 ± 0.0016**	**1.0227 ± 0.0016**	**1.0083 ± 0.0016**	**-0.0038**	**0.0227**	**0.0083**	**-0.0144**
83	**ydr14pl2**	**1.0026 ± 0.0015**	**1.0009 ± 0.0015**	**1.0175 ± 0.0014**	**1.0023 ± 0.0015**	**-0.0017**	**0.0166**	**0.0014**	**-0.0152**

Table II.2 (continued)

Case No.	Case Designation	k_eff ± σ				Δk			
		238-group (NITAWL-II Revised) (A)	238-group (NITAWL-III Revised) (B)	199g VITAMIN-B6 (BONAMI) (C)	199g VITAMIN-B6 ^{238}U-Multi-pole Parameters (NITAWL-III Revised) (D)	(B-A)	(C-B)	(D-B)	(D-C)
84	**ydr14pl3**	**1.0082 ± 0.0018**	**1.0056 ± 0.0017**	**1.0324 ± 0.0018**	**1.0166 ± 0.0021**	**-0.0026**	**0.0268**	**0.0110**	**-0.0158**
85	**ydr14un3**	**1.0147 ± 0.0018**	**1.0125 ± 0.0017**	**1.0382 ± 0.0016**	**1.0222 ± 0.0016**	**-0.0022**	**0.0257**	**0.0097**	**-0.0160**
86	or260901	1.0057 ± 0.0013	1.0057 ± 0.0013	1.0043 ± 0.0016	1.0056 ± 0.0016	0.0000	-0.0014	-0.0001	0.0013
87	or260906	1.0005 ± 0.0014	1.0024 ± 0.0014	1.0021 ± 0.0017	1.0025 ± 0.0013	0.0019	-0.0003	0.0001	0.0004
88	rfp2710u	1.0028 ± 0.0022	0.9987 ± 0.0025	1.0020 ± 0.0024	1.0046 ± 0.0022	-0.0041	0.0033	0.0059	0.0026
89	rfp2710r	1.0030 ± 0.0027	1.0007 ± 0.0024	c	c	-0.0023	N/A	N/A	N/A
90	or2968s1	0.9904 ± 0.0020	0.9888 ± 0.0018	0.9980 ± 0.0019	0.9938 ± 0.0017	-0.0016	0.0092	0.0050	-0.0042
91	or2968a1	1.0056 ± 0.0013	1.0056 ± 0.0013	1.0113 ± 0.0012	1.0049 ± 0.0012	0.0000	0.0057	-0.0007	-0.0064
92	or2968s2	0.9999 ± 0.0011	0.9995 ± 0.0011	1.0047 ± 0.0011	0.9999 ± 0.0010	-0.0004	0.0052	0.0004	-0.0048

a. ^{113}In (MAT: 49113) and ^{115}In (MAT: 49115) not in 199-group library.
b. ^{204}Pb (MAT: 82204) not in 199-group library.
c. ^{79}Br (MAT: 35079) and ^{81}Br (MAT: 35081) not in 199-group library.

III. POLIDENT

III.1 AMPX Upgrade

The module POLIDENT is used to access the resonance parameters in File 2 of an ENDF/B library, generate point cross sections and combine the cross sections with File 3 point data. POLIDENT is available in AMPX-77; however, the code could not process Version 6 evaluations of the ENDF system. With the AMPX upgrade, several modifications were made to enable processing of the new ENDF/B-VI formats.

One of the more significant modifications in POLIDENT involved the development of a new and innovative energy meshing technique for processing point data in the RRR. A discussion of the meshing scheme is provided in Reference 4. At the heart of any point cross-section processing code is the generation of a suitable energy mesh for representing the data. In the resonance region, the objective of a meshing scheme is to accurately represent the resonance structure with an efficient number of points. The development of a suitable grid in the resonance region is further complicated by the width and spacing of the resonances as well as interference effects from neighboring resonances. These factors can vary depending on the particular isotope under evaluation. Consequently, a suitable energy mesh is problem or isotope dependent.

With regard to NJOY, an energy mesh is constructed from a coarse grid which is based on the ENDF File 3 point data. During resonance reconstruction, additional points are added to the initial grid by halving each panel and inserting points until a desired convergence is achieved. This approach works well if the maximum error occurs at the midpoint of the panel. However, if the maximum error occurs at another point within an interpolation panel, the halving approach could miss an important energy point in the grid construction. As part of the POLIDENT upgrade, a new approach is implemented which is based largely on the determination of a very fine energy mesh. Subsequently, an auxiliary grid structure is determined by collapsing the number of points from the fine grid. The auxiliary grid structure is determined such that the original grid can be reproduced within a user specified tolerance, ε_{aux}.

Constructing the fine energy mesh is a very significant component of the meshing scheme. Initially, POLIDENT reads the File 2 resonance parameters and sub-divides the RRR into decade (i.e., 10 eV) intervals. Within each decade, the mean level spacing, $<D>$, and the mean neutron line width, $<\Gamma_n>$, are calculated. The initial estimate of the energy increment, ΔE, for each decade is given by the following relation:

$$\Delta E \ = \ C \ \frac{< \Gamma_n >}{< D >}. \qquad\qquad (1)$$

C = constant

Based on the initial estimate of ΔE, POLIDENT calculates the absorption, capture, fission, scattering and total cross sections using the ENDF specified functional representation (i.e., Reich-Moore, Single- and Multi-Level Breit Wigner). Use of the ENDF specified format provides a rigorous treatment of the cross- section data and accounts for interference effects which are induced by other resonance reactions. Using the calculated cross sections, the maximum, minimum and inflection points (i.e., critical points) are determined numerically for each reaction. A check is made to insure each resonance peak is present in the fine energy grid, and the resonance

energy points are added to the fine grid as needed. Additional points are added between the resonance peak and the points of inflection based on the slope between the two points.

To complete the fine grid determination, an iteration scheme is also used to add points until the fine grid cross sections are within a tolerance, ε_{fine}, of the actual cross-section data using linear interpolation. The fine grid tolerance is less than the desired auxiliary grid tolerance, ε_{aux}, (i.e., $0.1\varepsilon_{aux} \leq \varepsilon_{fine} < \varepsilon_{aux}$). Prior to the iteration scheme, the fine grid may have more than enough points to satisfy the ε_{fine} criterion in all or part of the RRR; however, the iteration scheme insures enough points are present in the fine grid such that the actual cross-section data can be reproduced to at least ε_{fine}. In other words, the maximum difference between the actual cross-section data and the fine grid is ε_{fine}. Once the iteration scheme is complete, the auxiliary grid is collapsed from the fine energy mesh. Initially, the critical points from the fine mesh calculation are transferred to the auxiliary grid. To complete the auxiliary grid construction, **each** fine grid cross-section value, $\sigma^{fine}(E)$, between critical points is linearly estimated using the critical points in the auxiliary grid. Fine grid points are added to the auxiliary grid until **each** fine grid cross-section value can be calculated within the desired convergence tolerance, ε_{aux}. Results obtained with the revised version of POLIDENT are presented in Section III.2.

III.2 TESTING

III.2.1 Comparisons with NJOY

As noted in Section III.1, POLIDENT is used to access the resonance parameters in File 2 of an ENDF/B library, generate point cross sections and combine the cross sections with File 3 point data. In an effort to test the code, continuous energy cross sections were calculated for ^{235}U. The POLIDENT generated cross sections are based on the ENDF/B-VI Release 5 evaluation for ^{235}U.[7] The total cross section as a function of energy is presented in Figure III.1 for ^{235}U at 0 K using POLIDENT with a convergence tolerance of 1%. With the new meshing scheme, the resulting energy grid for the total cross section in the RRR consists of 62,587 points. Since NJOY is the only production level code available to process ENDF/B-VI data, comparisons with NJOY can be used to evaluate the accuracy of POLIDENT. Using the same ENDF evaluation and reconstruction tolerance of 1%, cross sections obtained with NJOY97 are also presented in Figure III.1. The resulting energy grid from NJOY97 consists of 84,442 points in the RRR. Both codes were executed on CA38 which is a DEC Alpha AS 500/500 workstation in the Computational Physics and Engineering Division at ORNL. To compare the cross sections obtained with both codes, the ratio between the NJOY97 calculated cross sections and POLIDENT calculated cross sections is also provided in Figure III.1. As shown in Figure III.1, the difference in the data between 10.0 eV and 2.25×10^3 eV is within 1% which is consistent with the 1% convergence tolerance. It should be noted that similar agreement is observed from 1.0×10^{-5} eV to 10.0 eV.
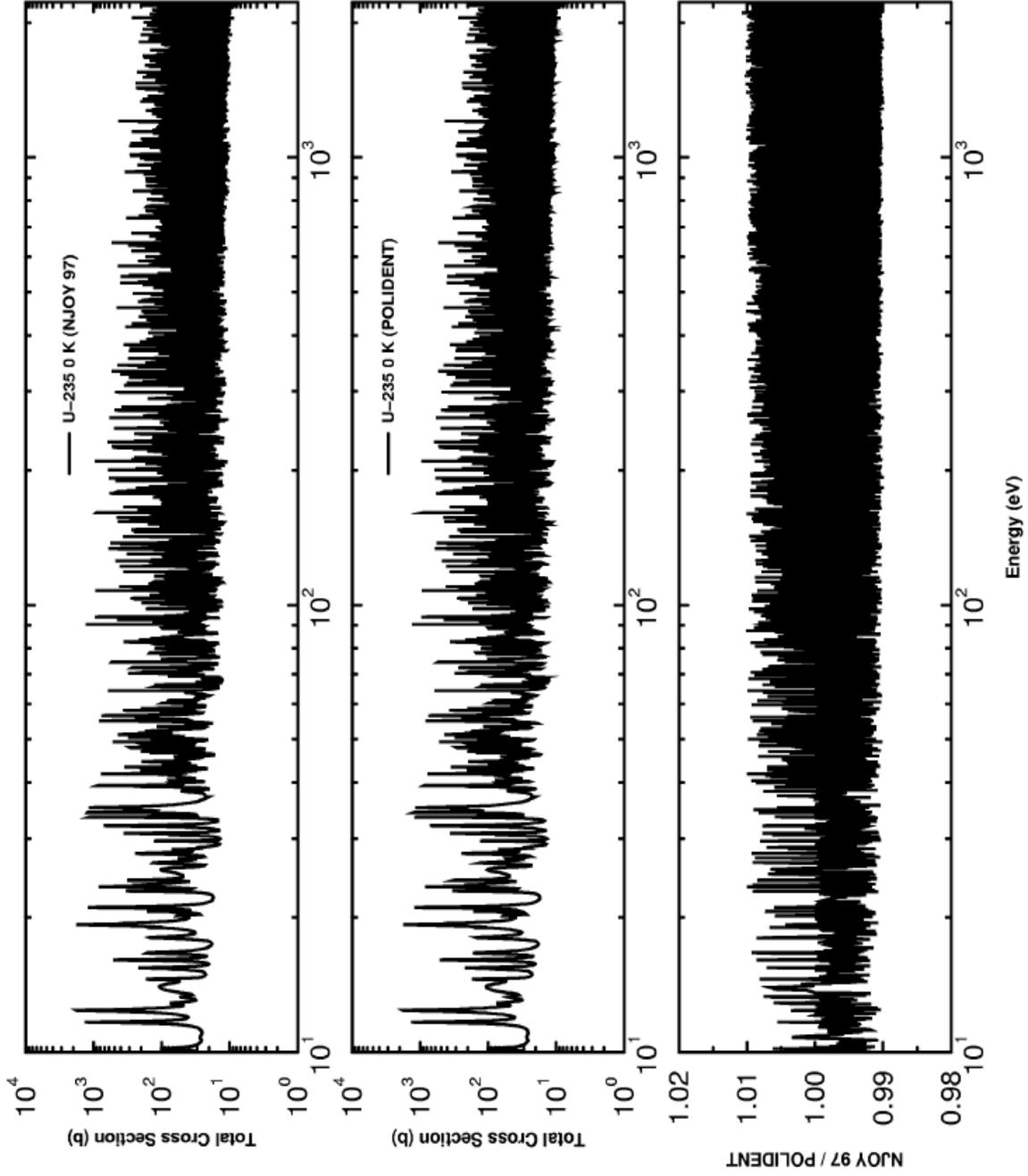
18

Figure III.1: Comparison of POLIDENT and NJOY97 Generated Total Cross Sections for ^{235}U as a Function of Energy.

19

III.2.2 Calculations with MCNP

Additional testing of POLIDENT generated cross sections in criticality safety calculations is presented in Reference 8. Although the work presented in Reference 8 will not be repeated in this report, the pertinent results are presented to sufficiently demonstrate the capabilities of POLIDENT. In particular, POLIDENT was used to generate continuous energy cross sections for 14 ENDF/B-VI isotopes at 0 K. Subsequently, the NJOY97 code system was used to process the POLIDENT data to 300 K and generate MCNP[9] cross sections for each isotope. A complete discussion of the cross-section generation process is provided in Reference 8. The prototypic AMPX/NJOY cross-section library was tested by calculating 21 KENO V.a test problems using MCNP.[10] For comparison, the 21 test cases were also calculated with the MCNP libraries which are distributed with MCNP. A brief description of each test case is provided in Table III.1, and the corresponding calculated results for the 21 problems are presented in Table III.2.

The differences in the calculated results are presented in the last column of Table III.2 (i.e., Column B-A). The calculated k_{eff} values obtained with the AMPX/NJOY97 generated cross sections agree with the results presented in Column (A); however, the calculated results for ksp_16 is ~1.4% less than the original MCNP library. The fissile material in ksp_16 consists of U(93.2)O_2F_2 solution with an H/X ~44. As discussed in Reference 8, the ^{235}U cross-section data provided with MCNP is based on ENDF/B-VI Release 2 data. In contrast, the AMPX/NJOY generated cross sections for ^{235}U are based on Release 5 data. Moreover, significant changes in the resonance data were made between Release 2 and Release 5 of the ENDF/B-VI evaluations. In particular, Release 2 capture cross-section values in the epithermal range were determined to be too small relative to the experimental measurements.[7] For example, in the energy range from 100 to 1000 eV the average capture cross section is 5.216 barns in ENDF/B-VI Release 2 as compared with 6.343 barns in Release 5 (i.e., 22% difference). Previous experimental measurements give average capture cross-section values of 6.33 and 6.18 barns from 100 to 1000 eV which agrees with the ENDF/B-VI Release 5 data.[7] Due to relatively low H/X ratio in ksp_16, the fissile system is not well moderated. Inspection of the neutron flux tally from the ksp_16 output reveals that the flux is peaked toward energies above 550 eV. Based on the neutron flux information and the differences between Release 2 and Release 5 data, the ~1.4% higher multiplication factor obtained with the original MCNP cross-section set can be attributed to the smaller capture cross-section values in the Release 2 data for ^{235}U relative to Release 5. In an effort to further evaluate the difference, MCNP cross sections were generated for ^{235}U using NJOY97 with ENDF/B-VI data (i.e., no AMPX contribution). Case ksp_16 in Column (A) was re-calculated with the original MCNP cross sections, except the original ^{235}U cross-section set was replaced with the ENDF/B-VI Release 5 data set generated by NJOY97. The calculated k_{eff} obtained with Release 5 ^{235}U cross-section data is 0.9875 ± 0.0022 which is within 0.5% of the value obtained using AMPX/NJOY97 cross sections. Based on these results, the ~1.4% difference observed for ksp_16 is attributed to the different Releases of ENDF/B-VI data for ^{235}U. Based on these results, the AMPX code system has the capability to process ENDF/B-VI data and generate independent cross sections for nuclear applications.

Table III.1: Description of 21 KENO V.a Test Problems[10]

Sample problem	Problem Description
ksp_1	Bare $2\times 2\times 2$ array of uranium metal cylinders
ksp_2	Same as problem 1 with different geometrical description and options
ksp_6	Single unit from problem 1
ksp_7	Single unit from problem 1 mirror reflected on x, y and z faces
ksp_8	Infinitely long metal cylinder from problem 1
ksp_9	$2\times 2\times 2$ array of uranium cylinders specularly reflected on all faces
ksp_10	Same as problem 1 with restart information written every 5th generation
ksp_11	Restart problem 10 with 51st generation
ksp_12	Array of four uranium metal cylinders and four cylinders of $UO_2(NO_3)_2$ solution
ksp_13	Two uranium metal cuboids in uranium metal annulus
ksp_14	Uranium metal cylinder in uranium metal annulus
ksp_15	Water reflected uranium metal sphere supported by plexiglass collar
ksp_16	Infinite number of slabs of $U(93.2)O_2F_2$ solution
ksp_17	Sphere of $U(93.2)O_2F_2$ solution
ksp_19	Same as problem 12 using array of arrays option
ksp_20	Triangular pitched array of 7 $U(93.2)O_2F_2$ cylinders
ksp_21	Unreflected sphere of $U(4.89)O_2F_2$ solution
ksp_22	Same as problem 1 with different geometrical description
ksp_23	Same as problem 1 with different geometrical description
ksp_24	Same as problem 1 with different geometrical description
ksp_25	Same as problem 1 with different geometrical description

Table III.2: MCNP Calculated Results for KENO V.a Test Problems
Using ENDF/B-VI Cross Sections Generated by POLIDENT/NJOY

| | Calculated $k_{eff} \pm \sigma$ | | |
Sample Problem	MCNP ENDF/B-VI[a] Cross-Section Set (ZAID.60c) (A)	ENDF/B-VI (AMPX/NJOY97)[b] (B)	Δk (B-A)
ksp_1	0.9957 ± 0.0017	0.9938 ± 0.0017	-0.0019
ksp_2	0.9957 ± 0.0017	0.9938 ± 0.0017	-0.0019
ksp_6	0.7410 ± 0.0014	0.7432 ± 0.0013	0.0022
ksp_7	0.9944 ± 0.0018	0.9969 ± 0.0018	0.0025
ksp_8	0.9350 ± 0.0016	0.9378 ± 0.0017	0.0028
ksp_9	2.2630 ± 0.0018	2.2589 ± 0.0021	-0.0041
ksp_10	0.9957 ± 0.0017	0.9938 ± 0.0017	-0.0019
ksp_11	0.9957 ± 0.0017	0.9938 ± 0.0017	-0.0019
ksp_12	1.0001 ± 0.0026	0.9966 ± 0.0028	-0.0035
ksp_13	0.9895 ± 0.0020	0.9899 ± 0.0019	0.0004
ksp_14	0.9974 ± 0.0018	0.9960 ± 0.0020	-0.0014
ksp_15	1.0001 ± 0.0023	0.9977 ± 0.0021	-0.0024
ksp_16	0.9964 ± 0.0022	0.9827 ± 0.0021	-0.0137
ksp_17	1.0023 ± 0.0029	1.0020 ± 0.0033	-0.0003
ksp_19	1.0001 ± 0.0026	0.9966 ± 0.0028	-0.0035
ksp_20	0.9966 ± 0.0032	0.9892 ± 0.0029	-0.0074
ksp_21	0.9927 ± 0.0019	0.9972 ± 0.0018	0.0045
ksp_22	0.9942 ± 0.0018	0.9921 ± 0.0018	-0.0021
ksp_23	0.9957 ± 0.0017	0.9938 ± 0.0017	-0.0019
ksp_24	0.9928 ± 0.0018	0.9920 ± 0.0018	-0.0008
ksp_25	0.9974 ± 0.0018	0.9961 ± 0.0017	-0.0013

[a]Thermal data based on ENDF/B-VI cross sections for H in H_2O is not available with the distributed MCNP library at the time of testing. Consequently, ENDF/B-V thermal data for H in H_2O is used as appropriate.

[b]C, ^{14}N and [16]O processed with POLIDENT and NJOY94. Also thermal data for H in H_2O processed by POLIDENT and NJOY94.

III. 2.3 Calculations with CENTRM and XSDRNPM

The Nordheim Integral Treatment is one of the current methods used in the SCALE system for resonance self-shielding calculations, and NITAWL is the SCALE module which generates resonance self-shielded cross sections for problem specific criticality safety calculations. The Nordheim Integral Treatment involves a solution for the energy dependence of the neutron flux in a material region containing a resonance absorber and a maximum of two admixed moderators. The presence of more than one absorber lump in the moderating medium (e.g., fuel pin lattice) is accounted through the use of a Dancoff factor.

The Nordheim Integral Treatment (i.e., NITAWL) is effective for the majority of criticality safety applications. However, there is a limited class of problems for which a different approach is required for the generation of resonance self-shielded cross sections. For instance, NITAWL is not suited for applications which have the resonance absorber appearing in more than one spatial zone (e.g., fuel dissolver solution geometries). Moreover, problems which have several resonance nuclides competing for the same slowing down source are not well suited for the approximations in NITAWL.

A new SCALE module named CENTRM has been developed to address the limitations associated with NITAWL.[12] CENTRM explicitly calculates a problem-dependent point flux from continuous energy cross sections which are produced by POLIDENT. The continuous energy flux spectrum is subsequently used to create problem-dependent multigroup cross sections using the code PMC.

In an effort to test CENTRM as well as demonstrate the capability to process ENDF/B-VI cross sections with POLIDENT, thirty test cases were calculated using CENTRM generated cross sections in criticality safety applications. The cases are based on the International OECD/NEA Criticality Working Group Benchmark 20 problem (Reference 13). These problems involve UO_2 fuel pellets which are partially dissolved in borated UO_2 solution.

The thirty test cases which are discussed in Reference 12 can be divided into five problem sets. The first set of problems is comprised of a triangular pitched assembly arranged on 1.0297 cm pitch with a 0.6 UO_2 volume fraction. In the second set, the cases have a 1.0943 cm triangular pitched assembly with a 0.5 UO_2 volume fraction. Likewise, the cases in the third set have a 1.1788 cm triangular pitched assembly with a 0.4 UO_2 volume fraction. The remaining cases are arranged on a rectangular pitch. In particular, the fourth set of problems has a 0.9749 cm pitch with a 0.5 UO_2 volume fraction, and the fifth set of problems has a 1.0501 cm pitch with a 0.4 UO_2 volume fraction.

Each set of problems has six cases where the amount of UO_2 in the pellet and boron concentration are varied. In particular, the cases that have an "a" or "b" designation contain 100% of the UO_2 in the pellet. The cases which are denoted with "c" and "d" have 75% UO_2 in the pellet with the remaining UO_2 in the surrounding solution. Likewise, the cases which are denoted with "e" and "f" have 50% UO_2 in the pellet with the balance in the surrounding solution. It should be noted that the cases denoted with "a", "c" and "e" have 3500 ppm Boron in the solution, and the cases denoted with "b", "d" and "f" have 1500 ppm Boron in the solution.

The calculated results are presented in Table III.3 for the thirty test problems. All the cases in Columns (a) and (b) are analyzed using BONAMI to process the unresolved resonance data and NITAWL-II to process the resolved resonance data. The 1-D discrete ordinates module XSDRNPM is subsequently used to calculate the system multiplication using the problem-dependent cross sections generated by BONAMI and

NITAWL. The results in Columns (a) and (b) are based on ENDF/B-V and -VI data, respectively. It should be noted that the ENDF/B-VI CENTRM library is used in conjunction with the 199-group VITAMIN/B-6 library for data outside the resolved resonance region. The thirty test problems are also analyzed using the new SCALE sequence: BONAMI, CENTRM, PMC and XSDRNPM. All cases involving CENTRM are presented in Columns (c) and (d). The results in Columns (c) and (d) are based on ENDF/B-V and -VI cross sections, respectively. The results presented in Columns (a) through (d) are compared to previously published calculations by Bernnat and Keinert which are presented in Column (e).[13] With regard to the Bernnat calculations, special care was taken to properly treat the resonances in the solution by calculating a fine mesh neutron spectrum over the RRR.

The calculated differences between the results obtained with the different resonance processors are presented in Table III.4. As noted in Table III.4, the NITAWL, CENTRM and Bernnat results with ENDF/B-V data for Cases 1a – 5a and 1b – 5b agree within 1%. Using ENDF/B-VI data, the NITAWL, CENTRM and Bernnat results agree within 1% for Cases 1a – 5a and 1b – 5b except for NITAWL Cases 4a and 5a. The NITAWL results for Cases 4a and 5a are within 2% of the Bernnat results. For the cases designated with an "a" identifier, 100% of the UO_2 is contained within the pellets, and the problem does not have double heterogeneity. Consequently, the uranium does not appear in additional spatial zones, and NITAWL provides good results for these cases. However, in the remaining cases which are designated "c" – "f", double heterogeneity is introduced into the resonance self-shielding calculation.

In the remaining cases (i.e., designation "c" – "f"), the UO_2 is also present in the solution which surrounds the pellets. Based on comparisons with the Bernnat results for the remaining cases, a significant improvement is obtained with the CENTRM results relative to NITAWL for both ENDF/B-V and -VI cross-section data. The Bernnat/CENTRM differences (absolute) using ENDF/B-V data for "c" – "f" case designations range between 1×10^{-4} and 0.0094. In comparison, the Bernnat/NITAWL differences range between 0.0208 and 0.0709 for the "c" – "f" case designations. With regard to ENDF/B-VI data, the Bernnat/CENTRM differences for Cases "c" – "f" range between 7×10^{-4} and 0.0136. Using ENDF/B-VI data for case "c" – "f" designations, the Bernnat/NITAWL differences range between 0.0075 and 0.0484.

Based on the results in Tables III.3 and III.4, CENTRM provides a significant improvement over NITAWL for processing resolved resonances in problems with resonance absorbers in more than one spatial zone. In addition, the results obtained with CENTRM using POLIDENT generated continuous energy cross sections agree with previously published benchmark values. Also, these results further demonstrate the capability of POLIDENT to generate continuous energy cross sections for criticality safety applications using ENDF/B-V and ENDF/B-VI data.

Table III.3: Calculated Results for the NITAWL-II and CENTRM Resolved Resonance Processors Using ENDF/B-V and ENDF/B-VI Data

Case	Wt % UO$_2$ in Pellet	Boron Conc. (ppm)	λ_∞				
			ENDF/B-V NITAWL (a)	ENDF/B-VI NITAWL (b)	ENDF/B-V CENTRM (c)	ENDF/B-VI CENTRM (d)	Previously Published Results (Bernnat) (e)
1a	100	3500	1.0132	1.0203	1.0086	1.0039	1.0099
1b	100	1500	1.1008	1.1084	1.0957	1.0907	1.0983
1c	75	3500	0.9323	0.9526	0.9891	0.9839	0.9924
1d	75	1500	1.0086	1.0311	1.0722	1.0667	1.0795
1e	50	3500	0.9284	0.9507	0.9843	0.9789	0.9881
1f	50	1500	1.0027	1.0274	1.0653	1.0596	1.0732
2a	100	3500	1.0022	1.0070	1.0002	0.9961	0.9955
2b	100	1500	1.1338	1.1392	1.1315	1.1271	1.1327
2c	75	3500	0.9330	0.9490	0.9770	0.9725	0.9744
2d	75	1500	1.0506	1.0690	1.1020	1.0971	1.1054
2e	50	3500	0.9299	0.9483	0.9726	0.9681	0.9704
2f	50	1500	1.0447	1.0658	1.0946	1.0897	1.0981
3a	100	3500	0.9474	0.9493	0.9463	0.9431	0.9443
3b	100	1500	1.1285	1.1305	1.1272	1.1236	1.1276
3c	75	3500	0.8917	0.9027	0.9221	0.9188	0.9166
3d	75	1500	1.0564	1.0696	1.0938	1.0901	1.0937
3e	50	3500	0.8900	0.9040	0.9194	0.9160	0.9142
3f	50	1500	1.0510	1.0679	1.0873	1.0835	1.0877
4a	100	3500	1.0039	1.0088	1.0002	0.9961	0.9930
4b	100	1500	1.1358	1.1412	1.1315	1.1271	1.1328
4c	75	3500	0.9331	0.9491	0.9770	0.9725	0.9732
4d	75	1500	1.0507	1.0691	1.1020	1.0971	1.1050
4e	50	3500	0.9295	0.9478	0.9726	0.9680	0.9699
4f	50	1500	1.0443	1.0653	1.0946	1.0896	1.0978
5a	100	3500	0.9481	0.9501	0.9464	0.9432	0.9337
5b	100	1500	1.1293	1.1314	1.1272	1.1237	1.1221
5c	75	3500	0.8919	0.9029	0.9221	0.9188	0.9127
5d	75	1500	1.0565	1.0697	1.0938	1.0901	1.0914
5e	50	3500	0.8898	0.9038	0.9195	0.9160	0.9113
5f	50	1500	1.0508	1.0676	1.0873	1.0835	1.0859

Table III.4: Calculated Differences Between NITAWL–II and CENTRM Resolved Resonance Processors Using ENDF/B-V and ENDF/B-VI Data

Case	Wt % UO$_2$ in Pellet	Boron Conc. (ppm)	$\Delta\lambda_\infty$					
			(CENTRM - NITAWL) ENDF/B-V	(CENTRM - NITAWL) ENDF/B-VI	(Bernnat - NITAWL) ENDF/B-V	(Bernnat - NITAWL) ENDF/B-VI	(Bernnat - CENTRM) ENDF/B-V	(Bernnat - CENTRM) ENDF/B-VI
1a	100	3500	-0.0046	-0.0164	-0.0033	-0.0104	0.0013	0.006
1b	100	1500	-0.0051	-0.0177	-0.0025	-0.0101	0.0026	0.0076
1c	75	3500	0.0568	0.0313	0.0601	0.0398	0.0033	0.0085
1d	75	1500	0.0636	0.0356	0.0709	0.0484	0.0073	0.0128
1e	50	3500	0.0559	0.0282	0.0597	0.0374	0.0038	0.0092
1f	50	1500	0.0626	0.0322	0.0705	0.0458	0.0079	0.0136
2a	100	3500	-0.002	-0.0109	-0.0067	-0.0115	-0.0047	-0.0006
2b	100	1500	-0.0023	-0.0121	-0.0011	-0.0065	0.0012	0.0056
2c	75	3500	0.044	0.0235	0.0414	0.0254	-0.0026	0.0019
2d	75	1500	0.0514	0.0281	0.0548	0.0364	0.0034	0.0083
2e	50	3500	0.0427	0.0198	0.0405	0.0221	-0.0022	0.0023
2f	50	1500	0.0499	0.0239	0.0534	0.0323	0.0035	0.0084
3a	100	3500	-0.0011	-0.0062	-0.0031	-0.005	-0.002	0.0012
3b	100	1500	-0.0013	-0.0069	-0.0009	-0.0029	0.0004	0.004
3c	75	3500	0.0304	0.0161	0.0249	0.0139	-0.0055	-0.0022
3d	75	1500	0.0374	0.0205	0.0373	0.0241	-0.0001	0.0036
3e	50	3500	0.0294	0.012	0.0242	0.0102	-0.0052	-0.0018
3f	50	1500	0.0363	0.0156	0.0367	0.0198	0.0004	0.0042
4a	100	3500	-0.0037	-0.0127	-0.0109	-0.0158	-0.0072	-0.0031
4b	100	1500	-0.0043	-0.0141	-0.003	-0.0084	0.0013	0.0057
4c	75	3500	0.0439	0.0234	0.0401	0.0241	-0.0038	0.0007
4d	75	1500	0.0513	0.028	0.0543	0.0359	0.003	0.0079
4e	50	3500	0.0431	0.0202	0.0404	0.0221	-0.0027	0.0019
4f	50	1500	0.0503	0.0243	0.0535	0.0325	0.0032	0.0082
5a	100	3500	-0.0017	-0.0069	-0.0144	-0.0164	-0.0127	-0.0095
5b	100	1500	-0.0021	-0.0077	-0.0072	-0.0093	-0.0051	-0.0016
5c	75	3500	0.0302	0.0159	0.0208	0.0098	-0.0094	-0.0061
5d	75	1500	0.0373	0.0204	0.0349	0.0217	-0.0024	0.0013
5e	50	3500	0.0297	0.0122	0.0215	0.0075	-0.0082	-0.0047
5f	50	1500	0.0365	0.0159	0.0351	0.0183	-0.0014	0.0024

IV. SUMMARY

The DOE Laboratory Project and Cost Proposal for NRC Work (JCN W6479) identifies various subtasks for upgrading the AMPX code system to process ENDF/B-VI data.[1] The overall objective of the upgrade is to facilitate independent processing of ENDF/B Version 6 formats. Two subtasks are identified in Task 6 of the cost proposal. In the first subtask, the AMPX system must be upgraded to allow production of continuous energy cross sections from ENDF Files 2 and 3 data. In the second subtask, the AMPX code system must be modified to incorporate the multi-pole formalism option for processing cross sections in the resolved resonance region. Prior to the release of the revised AMPX code system, comprehensive testing is needed to establish the capabilities of the new codes and procedures. Task 11 of the cost proposal specifies testing to verify the completion of the two subtasks. In accordance with the reporting requirements for Task 11, this report documents the development and testing associated with the production of continuous energy cross sections and the processing of multi-pole resonance parameters.

The AMPX module POLIDENT has been modified to process ENDF/B Version 6 formats and to generate infinite dilution cross-section values. With regard to multi-pole processing, the master library format has been revised to permit the storage of double precision multi-pole parameters in the existing single precision format.   By maintaining the existing AMPX master library format, many SCALE and AMPX codes which read an AMPX master library do not require modification. To enable multi-pole processing, a new code (i.e., KRYSTAL) has been developed to calculate the multi-pole parameters from the ENDF data. Subsequently, a new version of NITAWL (i.e., NITAWL-III) has been developed to process the multi-pole parameters and calculate self-shielded cross sections in the resolved resonance region.

In an effort to establish the capabilities of POLIDENT, continuous energy cross sections were generated for ^{235}U at 0 K using ENDF/B-VI data. The POLIDENT generated cross sections were subsequently compared with NJOY calculated cross sections on a point-by-point basis. The differences between NJOY and POLIDENT are within $\pm$ 1% which is consistent with the convergence tolerance used in the energy mesh generation.

With regard to criticality safety applications, POLIDENT was used to generate cross sections for 14 ENDF/B-VI isotopes/nuclides at 0 K. Subsequently, the NJOY code system was used to process the AMPX cross-section data to 300 K and generate MCNP cross sections for each isotope/nuclide. The prototypic cross-section library was tested by calculating twenty-one KENO V.a test problems using MCNP. For comparison, the twenty-one test problems were calculated with the ENDF/B-VI MCNP libraries which are distributed with the code. The calculated results obtained with the prototypic libraries agree with the calculated results obtained with the MCNP cross-section library. Based on these results, the AMPX code system can generate continuous energy cross sections using ENDF/B-VI data.

POLIDENT continuous energy cross sections based on ENDF/B-V and -VI data were also generated for use in CENTRM, the new resolved resonance processing module. CENTRM performs an explicit calculation of the problem-dependent point flux from continuous energy cross sections which are produced by POLIDENT. The continuous energy flux spectrum is subsequently used to create problem-dependent multigroup cross sections using the code PMC. Thirty test cases which involve UO_2 fuel pellets that are partially dissolved in borated UO_2 solution were examined using CENTRM/PMC and XSDRNPM. The calculated results obtained with CENTRM cross sections agree with the benchmark values for both ENDF/B-V

27

and -VI data. These results also demonstrate the capability of POLIDENT to generate continuous energy cross sections for criticality safety applications using ENDF/B-V and ENDF/B-VI cross sections.

Regarding NITAWL-III testing, 77 critical experiments were calculated using CSAS25 in an effort to test NITAWL-III. Using the 238-group ENDF/B-V library, the 77 critical experiments were calculated using NITAWL-II and -III generated cross sections. The calculated k_{eff} values obtained with NITAWL-III self-shielded cross sections are within two standard deviations of the results obtained with NITAWL-II. These results demonstrate that the capabilities of NITAWL-II are maintained in the latest version of NITAWL.

Previous criticality calculations using the 199-group VITAMIN-B6 library in SCALE/CSAS25 identified calculational problems for seven low-enriched thermal homogeneous systems with H/U values below 8.[5] The poor results are attributed to the narrow resonance approximation in the generation of self-shielded cross sections for ^{238}U in the resolved resonance region. In an effort to test the multi-pole capability, pole parameters were generated for ^{238}U, and a revised version of ^{238}U was added to the 199-group library. Using the revised 199-group cross-section library with multi-pole parameters leads to calculated k_{eff} values that are consistent with the calculated system multiplication obtained with the 238-group ENDF/B-V library. Based on these results, the AMPX code system can be used to generate and process multi-pole parameters for criticality safety applications.

V. REFERENCES

1. "Development and Applicability of Criticality Safety Software for Licensing Review," DOE Laboratory Project and Cost Proposal for NRC Work, JCN W6479, (January 22, 1999).

2. N. M. Greene, W. E. Ford III, L. M. Petrie, and J. W. Arwood, *AMPX-77: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Cross-Section Libraries from ENDF/B-IV and ENDF/B-V*, ORNL/CSD/TM-283, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, (October 1992).

3. R. E. MacFarlane and D. W. Muir, *NJOY97.0 Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data*, PSR-68 NJOY97.0, Los Alamos National Laboratory, (April 1998).

4. M. E. Dunn, N. M Greene and L. C. Leal, "Energy Meshing Techniques for Processing ENDF/B-VI Cross Sections Using the AMPX Code System," *Trans. Am. Nucl. Soc.*, (to published June 1999).

5. S. M. Bowman, R. Q. Wright, M. D. DeHart, C. V. Parks and L. M. Petrie, "Recent Validation Experience with Multigroup Cross-Section Libraries and SCALE," *ICNC '95 Fifth International Conference on Nuclear Criticality Safety*, Albuquerque, NM, **2**, 2•44 – 2•55, (September 17–21, 1995).

6. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2/R5), Vols I–III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

7. L. C. Leal, H. Derrien, N. M. Larson and R. Q. Wright, *R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 to 2.25 keV*, ORNL/TM-13516, Oak Ridge National Laboratory, (November 1997).

8. M. E. Dunn, *Production of MCNP Cross Sections Using the AMPX and NJOY Processing Code Systems*, ORNL/M-6609, (October 1998).

9. "MCNP 4A: Monte Carlo N-Particle Transport Code System," Los Alamos National Laboratory LA-12625-M, (November 1993).

10. L. M. Petrie and N. F. Landers, "KENO V.a: An Improved Monte Carlo Criticality Program with Supergrouping," Vol. 2, Sect. F11, of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2/R5), Vols I–III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

11. R. N. Hwang, "A Rigorous Pole Representation of Multilevel Cross Sections and Its Practical Applications," *Nuc. Sci. Eng.*, **96**, 192 (1987).

12. D. F. Hollenbach and L. M. Petrie, "Comparison of the CENTRM Resonance Processor to the NITAWL Resonance Processor in SCALE," *Trans. Am. Nucl. Soc.*, **78**, 158–159 (June 1998).

13. W. Bernnat, J. Keinert, "Calculation of the Benchmark 20 of the OECD-NEAWorking Group on Criticality Calculations," KfK 4695, IKE 6-180, Kernforschungszentrum Karlsruhe GmbH, Federal Republic of Germany (March 1990).

Appendix A

AMPX Master Library Resonance Parameter Data Format

AMPX Master Library Resonance Parameter Data Format

Two kinds of resolved resonance data can be placed on an AMPX Master library: the traditional Breit-Wigner data or the multi-pole data. All data for a nuclide are collected in one record, and all parameters in the record are "real" as opposed to integer values. Note that knowledge of the resonance parameter formats is not required for a SCALE or AMPX user. The formats are automatically interpreted by the codes that process the resonance parameters, and the following discussion is provided to document the details of the formats.

The same record structure is used for Breit-Wigner and multi-pole data as described below:

Table A.1: Overview of Data Blocks for Resonance Parameter Data

Data Block	Description
1.	Header Block consisting of 9 words
2.	Directory Control Block for Resonance Parameter Information
3.	Directory for Resonance Parameter Information
4.	Resonance Parameter Information

Formats for Breit-Wigner Resonance Parameters

A complete overview of the Breit Wigner data structure is provided in Table A.2.

1. Header Block

The header block consists of 9 words as follows:

1. **A**, the mass ratio for the isotope or element;
2. **SIGP0**, the potential scattering cross section;
3. **NLIB**, the library "number" or source of the data;
4. **NSIX**, the number of six-word groups needed to contain the resonance data. This is the value reported in the 20th word in the AMPX master library directory record for the nuclide;
5. **S**, a factor used in the mesh determination scheme in the Nordheim Integral Treatment. It is normally given a value of 0.0, which causes it to use an internal default;
6. **NMOD**, the "mod" number associated with the ENDF/B evaluation;
7. **NFOR**, the ENDF/B format level of the original data;
8. **NVER**, the "version" of the ENDF/B library from which the parameters are taken; and
9. **RTYPE**, the type of data in the record—0.0 for SLBW/MLBW parameters or 100.0 for multi-pole parameters.

(Note that words 3, 6, 7, and 8 above are normally zero in existing libraries, and have been activated to provide a means of identifying the source of the data that are included in the AMPX data set).

The format for Breit Wigner-data is provided in the following discussion. For the Breit Wigner case, every collection of information is arranged in 6 word groups, and all data are real numbers including the variables that are used as "counters."

2. Breit-Wigner DIRECTORY Control Block

The control block consists of 6 words which describes the structure of the following resonance data.

1. 0.0—this zero is used to indicate that the resonance parameter data are not in the original data format;
2. **NBLK**—the number of blocks of resonance parameter data which are given. Resonance parameter data are blocked to allow several situations, including different energy ranges over which a group of parameters are to be used, different isotopes, different l-states, etc.;
3. 0.0—this parameter is not used;
4. 0.0—this parameter is not used;
5. **TEMP**—the reference temperature at which the infinite dilution cross sections are calculated in the group averaged data in the library; and
6. 0.0—this parameter is not used.

3. Breit-Wigner DIRECTORY for Resonance Parameter Information

The data directory consists of NBLK groups of 6 words as follows:

1. **AWR**—the mass ratio for the isotope for the block,
2. **ABUN**—the abundance of the isotope,
3. **NRES**—the number of resonances in the block,
4. **L**—the l-value for the block,
5. **EL**—the low energy of the region where the resonances in this block should be used, and
6. **EH**—the high energy of the region where the resonances in this block should be used.

The first 6 words apply for the first block, the next 6 for the second block, etc.

4. Breit-Wigner RESONANCE DATA

Breit-Wigner resonance data are given in groups of 6 words, and are all blocked together. The first 6 times NRES words are for the first block, etc. The resonance parameter format is provided in the following description.

1. **E0**—the resonance energy,
2. Γ_n –the neutron width for the resonance,
3. Γ --the gamma width for the resonance,
4. Γ_f –the fission width for the resonance,
5. **R**—a factor used in determining the point value reconstruction array for the resonance, and
6. g_j –the statistical weight parameter for the resonance.

Table A.2: AMPX Master Library Structure for Breit Wigner Resonance Parameter Data

Information Type	Word 1	Word 2	Word 3	Word 4	Word 5	Word 6
Control Block	0.0	NBLK	0.0	0.0	TEMP	0.0
Data Directory	AWR_1	$ABUN_1$	$NRES_1$	L_1	EL_1	EH_1
	AWR_2	$ABUN_2$	$NRES_2$	L_2	EL_2	EH_2
	AWR_3	$ABUN_3$	$NRES_3$	L_3	EL_3	EH_3
	.					
	.					
	.					
	AWR_{NBLK}	$ABUN_{NBLK}$	$NRES_{NBLK}$	L_{NBLK}	EL_{NBLK}	EH_{NBLK}
Resonance Parameter Data for 1st Block	E0	Γ_n	Γ	Γ_f	R	g_j
	.					
	.					
	.					
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	.					
Resonance Parameter Data for 2nd Block	E0	Γ_n	Γ	Γ_f	R	g_j
	.					
	.					
	.					
	.					
	.					
Resonance Parameter Data for NBLK Block	E0	Γ_n	Γ	Γ_f	R	g_j

Multi-pole Resonance Parameter Format

As noted in Section II.1.1, the parameters for a pole consist of complex numbers that have values for "energy", "scattering cross section", "capture cross section", and "fission cross section". Since these 4 terms are complex, 8 parameters are required per pole. Two poles are required per resonance. Furthermore, the two poles are used in complicated calculations that require taking the difference of two numbers that could be very small (i.e., outside the limits of single-precision values). Consequently, a double precision format is needed to calculate accurate cross section values.

In the Breit Wigner format, resolved resonance parameters are stored in groups of 6-words per resonance, and the data directory for a nuclide tells how many of these 6-word groups are written. Clearly, more than 6 words are required to represent the data for a single pole.

A pseudo double precision scheme was developed for representing the multi-pole parameters in the existing single precision format. The pseudo double precision format is outlined in Section II.1.1. With regard to storage requirements, each pole requires 8 parameters, and the pseudo-double precision scheme requires 16 words to store the 8 parameters. Since there are two poles per resonance, the storage requirements for the multi-pole parameters for a resonance are 32 words.

As noted in Section II.1.1, the Reich-Moore parameters that were used to produce the pole parameters are also stored in the AMPX master library. The Reich-Moore parameters consist of the resonance energy, a total width, a scattering width, a gamma width, and two fission width terms. Consequently, each pole requires 6 additional words of data to be stored. (Note that the spin and angular momentum terms will be stored elsewhere in the formats such that they apply to a group of resonances and are not stored for individual resonances). By including the Reich-Moore data the storage requirements for a resonance increase to 38 words. Therefore, an arbitrary value of 20 words per pole is used in the AMPX resonance parameter format, and the Reich-Moore parameters are stored in the 4 extra words available in each pole. The resolved resonance parameter format for the multi-pole parameters is provided in the following description.

1. Header Block

The header block consists of 9 words as follows:

1. **A**, the mass ratio for the isotope or element,
2. **SIGP0**, the potential scattering cross section,
3. **NLIB**, the library "number" or source of the data,
4. **NSIX**, the number of six-word groups needed to contain the resonance data. This is the value reported in the 20th word in the AMPX master library directory record for the nuclide,
5. **S**, a factor used in the mesh determination scheme in the Nordheim Integral Treatment. It is normally given a value of 0.0, which causes it to use an internal default,
6. **NMOD**, the "mod" number associated with the ENDF/B evaluation,
7. **NFOR**, the ENDF/B format level of the original data,
8. **NVER**, the "version" of the ENDF/B library from which the parameters are taken, and

9. **RTYPE**, the type of data in the record—0.0 for SLBW/MLBW parameters or 100.0 for multi-pole parameters.

(Note that words 3, 6, 7, and 8 above are normally zero in existing libraries, and have been activated to provide a means of identifying the source of the data that are included in the AMPX data set).

2. Directory Control Block for Multi-pole Resolved Resonance Data

As mentioned earlier, the same structure used for the Breit-Wigner data is used for the multi-pole data. As a result, all types of data are blocked in 20 word groups. In the control block the words are defined as follows:

1. 0.0—this word is zero, as in the case of Breit-Wigner data,
2. **NBLK**, number of blocks of data that are given,
3. 0.0—this word is not used,
4. 0.0—this word is not used,
5. **TEMP**, the temperature in Kelvin at which the infinite dilution group-averaged cross sections were calculated and reported elsewhere in the file.
6. **NWLINE**, number of words per line of data. This parameter will be zero in existing libraries and will be defaulted to 6. It will be 20 for multi-pole data.

For the multi-pole case, all data blocks are divided into 20 word groups. Consequently, words 7-20 in this control block must be padded with zeroes.

3. Directory Block for Multi-pole Parameter Data

The next NBLK groups of NWLINE=20 words constitute a directory of the multi-pole parameter data.

1. **AWR**, the mass ratio for the isotope or element,
2. **ABUN**, the abundance if this is a multi-isotope evaluation, or 1.0 otherwise,
3. **NPOLES**, the number of poles in this block,
4. **LVAL**, the l-value (angular momentum) for this block,
5. **EL**, the lower energy cutoff for which the parameters in this block should be applied,
6. **EH**, the upper energy cutoff for which the parameters in this block should be applied,
7. **AJ**, the J value for the resonances in the block,
8. **SPIN**, the spin value for the resonances in the block,
9. **AP**, the scattering radius for the block,
10. **ZA**, the Z-number of the isotope multiplied by 1000 plus the A number for the isotope for the block,

As in the case of the directory control block, 20 word groups are used for the multi-pole case. As a result, words 11-20 in each line of the directory must be padded with zeroes.

4. **Multi-pole Parameter Data**

For the multi-pole case, the parameters are complex numbers that use two single precision words for the real and imaginary parts. As noted above, 16 words are required to represent a single pole. The 16 word representation for a single pole is arranged in the following format:

1. First word for the real part of the energy parameter of the resonance pole,
2. Second word for the real part of the energy parameter of the resonance pole,
3. First word for the imaginary part of the energy parameter of the resonance pole,
4. Second word for the imaginary part of the energy parameter of the resonance pole,
5. First word for the real part of the scattering parameter,
6. Second word for the real part of the scattering parameter,
7. First word for the imaginary part of the scattering parameter,
8. Second word for the imaginary part of the scattering parameter,
9. First word for the real part of the fission parameter,
10. Second word for the real part of the fission parameter,
11. First word for the imaginary part of the fission parameter,
12. Second word for the imaginary part of the fission parameter,
13. First word for the real part of the n-gamma parameter,
14. Second word for the real part of the n-gamma parameter,
15. First word for the imaginary part of the n-gamma parameter,
16. Second word for the imaginary part of the n-gamma parameter.

For the first pole of a resonance, four of the Reich-Moore parameters are stored in words 17 through 20.

17. E0, the resonance energy,
18. GT, the Reich-Moore total width,
19. GN, the Reich-Moore neutron width,
20. GG, the Reich-Moore gamma width.

The remaining two Reich-Moore parameters are stored with the data for the second pole of a resonance.

17. GFA, the first Reich-Moore fission width,
18. GFB, the second Reich-Moore fission width,
19. 0.0,
20. 0.0.

An overview of the AMPX Master library structure for words 1 through 10 is provided in Table A.3, and an overview for words 11 through 20 is provided in Table A.4.

Table A.3: AMPX Master Library Structure for the Multi-pole Resonance Data (words 1-10).

Data Type	Word 1	Word 2	Word 3	Word 4	Word 5	Word 6	Word 7	Word 8	Word 9	Word 10
Control Block	0.0	NBLK	0.0	0.0	TEMP	NWLINE	0.0	0.0	0.0	0.0
Data Directory	AWR_1	$ABUN_1$	$NPOLES_1$	L_1	EL_1	EH_1	J_1	$SPIN_1$	AP_1	ZA_1
	AWR_2	$ABUN_2$	$NPOLES_2$	L_2	EL_2	EH_2	J_2	$SPIN_2$	AP_2	ZA_2
	. . .									
	AWR_{NBLK}	$ABUN_{NBLK}$	$NPOLES_{NBLK}$	L_{NBLK}	EL_{NBLK}	EH_{NBLK}	J_{NBLK}	$SPIN_{NBLK}$	AP_{NBLK}	ZA_{NBLK}
Multi-pole Resonance Parameter Data for 1ˢᵗ Block	E1(real,1)	E1(real,2)	E1(imag,1)	E1(imag,2)	S1(real,1)	S1(real,1)	S1(imag,1)	S1(imag,2)	F1(real,1)	F1(real,2)
	E2(real,1)	E2(real,2)	E2(imag,1)	E2(imag,2)	S2(real,1)	S2(real,1)	S2(imag,1)	S2(imag,2)	F2(real,1)	F2(real,2)
	. . .									
	E1(real,1)	E1(real,2)	E1(imag,1)	E1(imag,2)	S1(real,1)	S1(real,1)	S1(imag,1)	S1(imag,2)	F1(real,1)	F1(real,2)
Multi-pole Resonance Parameter Data for 2ⁿᵈ Block	E2(real,1)	E2(real,2)	E2(imag,1)	E2(imag,2)	S2(real,1)	S2(real,1)	S2(imag,1)	S2(imag,2)	F2(real,1)	F2(real,2)
	. . .									
	E1(real,1)	E1(real,2)	E1(imag,1)	E1(imag,2)	S1(real,1)	S1(real,1)	S1(imag,1)	S1(imag,2)	F1(real,1)	F1(real,2)
Multi-pole Resonance Parameter Data for NBLK Block	E2(real,1)	E2(real,2)	E2(imag,1)	E2(imag,2)	S2(real,1)	S2(real,1)	S2(imag,1)	S2(imag,2)	F2(real,1)	F2(real,2)
	. . .									

Table A.4: AMPX Master Library Structure for the Multi-pole Resonance Data (Words 11-20).

Data Type	Word 11	Word 12	Word 13	Word 14	Word 15	Word 16	Word 17	Word 18	Word 19	Word 20
Control Block	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Data Directory	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
⋮										
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Multi-pole Resonance Parameter Data for 1st Block	F1(imag,1)	F1(imag,2)	C1(real,1)	C1(real,2)	C1(imag,1)	C1(imag,2)	E0	Γ_t	Γ_n	Γ
	F2(imag,1)	F2(imag,2)	C2(real,1)	C2(real,2)	C2(imag,1)	C2(imag,2)	Γ_{f1}	Γ_{f2}	0.0	0.0
⋮										
Multi-pole Resonance Parameter Data for 2nd Block	F1(imag,1)	F1(imag,2)	C1(real,1)	C1(real,2)	C1(imag,1)	C1(imag,2)	E0	Γ_t	Γ_n	Γ
	F2(imag,1)	F2(imag,2)	C2(real,1)	C2(real,2)	C2(imag,1)	C2(imag,2)	Γ_{f1}	Γ_{f2}	0.0	0.0
⋮										
Multi-pole Resonance Parameter Data for 2nd Block	F1(imag,1)	F1(imag,2)	C1(real,1)	C1(real,2)	C1(imag,1)	C1(imag,2)	E0	Γ_t	Γ_n	Γ
	F2(imag,1)	F2(imag,2)	C2(real,1)	C2(real,2)	C2(imag,1)	C2(imag,2)	Γ_{f1}	Γ_{f2}	0.0	0.0
⋮										

*In the preceding two tables, E1(real,1) is the first single precision real component of the first pole energy variable for a resonance; E1(real,2) is the second real single precision word; E1(imag,1) is the first single precision imaginary component, etc.; S is the symbol for the scattering residue term; F is the symbol for the fission residue term; and C is the symbol for the capture residue term.

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