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MCNP6 Computational-Based Sensitivity Propagation Analysis of Continuous Neutron Cross-Sections Using the Godiva (HMF-001) and the Godiver (HMF-004) Benchmark Criticality Study Cases

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MCNP6 COMPUTATIONAL-BASED SENSITIVITY PROPAGATION ANALYSIS OF
CONTINUOUS NEUTRON CROSS-SECTIONS USING THE GODIVA
(HMF-001) AND THE GODIVER (HMF-004) BENCHMARK
CRITICALITY STUDY CASES

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ABSTRACT

MCNP6 COMPUTATIONAL-BASED SENSITIVITY PROPAGATION ANALYSIS OF CONTINUOUS NEUTRON CROSS-SECTIONS USING THE GODIVA (HMF-001) AND THE GODIVER (HMF-004) BENCHMARK CRITICALITY STUDY CASES

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There has been a reduction in funding for theoretical and applied research for improving the nation's database of continuous neutron cross-sections at BNL-NNDC. From 1940 through the late 1980s, research and applied development produced volumes of reliable neutron continuous cross-sections for many isotopes. Currently, the cross-section work has been mainly computational. The focus of this research is mainly centered on the requirements for improving thermal cross-sections to support reactor operations and fuel storage. The research efforts will also helpfully aid in the fast fission spectrum in order to support fast reactor designs for improving safety analysis and feedback coefficients.

This previous level of effort produced well-defined sets of neutron cross-sections for a few applications, but only incidental information for outside of the desired range of the energy

spectrum. Isotope cross-sections are generally characterized from the isotope's fission energy to the thermal absorption energy, but not in as much detail outside of this roughly 0-3 MeV range. The good news is that each version of ENDF has improved the data points between the resolved resonance and hard sphere ranges.

The amount of characterization for an isotope's cross-section is determined by the number of experiments conducted. The sensitivity is then assigned to an isotope is after evaluation of the series of experiments are conducted and analyzed. If two isotopes were in a given experiment, then the cross-sections from the two isotopes will need to be separated or de-convoluted. Obtaining well-defined neutron cross-sections means that the sensitivity should be on the same order of magnitude through the entire range of the energy spectrum. This will require pure isotope foils for many of the experiments that will require de-convoluting the multiple cross-sections. Many observations will be required to uniformly reduce the sensitivity across the energy spectrum for each isotope.

The scope of this dissertation is to ascertain the quality of the uncertainties in the NNDC database for U-234, U-235, U-236, and U-238. This will aid in determining where the uncertainties are large and require additional future research. A comparison will be conducted to analyze the sensitivities through computational methodology, based on Monte Carlo particle transport code (MCNP6) with modern continuous-energy neutron data libraries (ENDF/B-VII.1). The Godiva HMF-001 and Godiver the water-reflected sphere HMF-004 criticality safety evaluation benchmark models will be used in the analysis.

A created Fortran program will modify the ENDF/B-VII cross-sections, and then standard Type I ACE cross-sections files will be generated using NJOY2012.50. By applying the perturbation to the cross-sections, in increasing increments, the change in K_{eff} will be calculated

in MCNP6 and MCNPX, and thus the amount of sensitivity can be determined when K_{eff} varies from the baseline. The difference in K_{eff} can be determined by modeling the two criticality benchmark experiments, through computationally-based analysis.

The perturbations applied to the two benchmarks will demonstrate the effect of the change in sensitivity on the overall bias of the safety analysis. In order to develop safe and reliable designs for fast fission reactors, transmutation and accelerator driven systems, additional research work will need to be conducted to improve the sensitivity for a larger range of energies. This will be coupled with work in uncertainty and feedback coefficients for NRC safety requirements.

This dissertation is to aid in showing where there are gaps in the sensitivities in the isotopes, as well as any correlations between the sensitivity and the change in K_{eff} . The long-term objective is that the developed data will allow quantifying models in a more rigorous manner, for the neutron cross-section related sensitivities in the calculated effective multiplication factor. This in turn should make a drive for an overall strategy for independent quality checks in criticality and reactivity analysis. This will improve the scientific basis for criticality safety analysis and increase the quality of the predictive capabilities, a necessary requirement in the possibility of establishing less conservative but more reliable regulatory safety criteria.

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P.S. Rajah, the ball is now in your court!

P.P.S. Dr. Sanchez, you were right...

TABLE OF CONTENTS

ABSTRACT	iii
ACKNOWLEDGEMENTS	vi
TABLE OF CONTENTS	vii
LIST OF TABLES	ix
LIST OF FIGURES	x
LIST OF ABBREVIATIONS	xi
CHAPTER 1: INTRODUCTION	1
CHAPTER 2: REVIEW OF RELATED LITERATURE.....	11
CHAPTER 3: METHODOLOGY	32
CHAPTER 4: FINDINGS OF THE STUDY	57
CHAPTER 5: SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS.....	68
APPENDIX A: ENDF FILE FORMATTING	70
APPENDIX B: NJOY LICENSE	71
APPENDIX C: MCNP6/X LICENSE	72
APPENDIX D: ENDF_MODIFY CODE	73
APPENDIX E: NJOY2012 DOS BATCH FILE	81
APPENDIX F: NJOY2012 DAT FILES	82
APPENDIX G: MASTER NJOY DOS BATCH FILE	86
APPENDIX H: NJOY2012 CROSS-SECTION PLOTS	87

APPENDIX I: XSDIR FILE	91
APPENDIX J: MCNP6/X INPUT FILES	92
APPENDIX K: MCNP6/X DOS BATCH FILES.....	94
APPENDIX L: ENDF/B EVOLUTION.....	96
BIBLIOGRAPHY	97
CURRICULUM VITAE	102

LIST OF TABLES

Table 1: NLIB Numbers.....	14
Table 2: NSUB-library Numbers and Names	14
Table 3: Material File (MF) Numbers and Names	15
Table 4: Material Type (MT) Numbers, Reactions, and Names	16
Table 5: Modules of NJOY	19
Table 6: Sections of ENDF Required for the Modules of NJOY	21
Table 7: Label Extensions for the Twelve Sets of Cross-Sections.....	35
Table 8: ENDF File Contents.....	41
Table 9: ENDF Material File 3/MT Structure.....	45
Table 10: Perturbed ENDF File	47
Table 11: Comparison of Benchmarks from MCNP6.....	58
Table 12: Comparisons of Benchmarks from MCNPX	59
Table 13: Slopes of Perturbation Amount to Increase in K_{eff}	60

LIST OF FIGURES

Figure 1: Example of ENDF File Formatting.....	17
Figure 2: ENDF File Data Contents.....	18
Figure 3: Directory Structure	36
Figure 4: NNBL ENDF Webpage for U-234	38
Figure 5: NNBL ENDF Webpage for U-235	39
Figure 6: NNBL ENDF Webpage for U-236	39
Figure 7: NNBL ENDF Webpage for U-238	39
Figure 8: ENDF Baseline Energy-Vs-Cross-sections graph for U-234.....	42
Figure 9: ENDF Baseline Energy-Vs-Cross-sections graph for U-235	43
Figure 10: ENDF Baseline Energy-Vs-Cross-sections graph for U-236.....	43
Figure 11: ENDF Baseline Energy-Vs-Cross-sections graph for U-238.....	44
Figure 12: Opening screen of ENDF_ModifyV106.exe.....	49
Figure 13: Completed ENDF_ModifyV106.exe Screen.....	49
Figure 14: MCNP6\X Comparisons for Perturbations.....	61
Figure 15: Neutron Facts from HMF-001 and HMF-004 at +30%	62
Figure 16: Neutron Spectrum in HMF-001	63
Figure 17: Neutron Spectrum in HMF-004	64

LIST OF ABBREVIATIONS

ACER	NJOY MODULE TO PRODUCE MCMP DATA LIBRARY
AEC	ATOMIC ENERGY COMMISSION
AENCF/AFGE	AVERAGE ENERGY OF NEUTRONS CAUSING FISSION
Am	AMERICIUM
ANL	ARGONNE NATIONAL LABORATORY
AWR	ATOMIC WEIGHT RATIO
BNL	BROOKHAVEN NATIONAL LABORATORY
BROADR	NJOY MODULE TO ADD TEMPERATURE DEPENDANCE TO POINTWISE CROSS SECTIONS
BWR	BOILING WATER REACTOR
CL	CRITICAL LIMIT
CLI	COMMAND LINE INTERFACE
Cm	CURIUM
cm	CENTIMETER
DAF	DEVICE ASSEMBLY FACILITY
DOE	DEPARTMENT OF ENERGY
EALF	ENERGY OF AVERAGE LETHARGY CAUSING FISSION
ENDF	EVALUATED NUCLEAR DATA FILES
ENDF/B	EVALUATED NUCLEAR DATA FILES/B FORMAT
g	GRAM
GASPR	NJOY MODULE FOR PRODUCING GAS PRODUCTION DATA

GENDF	GROUPWISE EVALUATED NUCLEAR DATA FILES
GLLSM	GENERAL LINEAR-LEAST SQUARES METHODS
HEATR	NJOY MODULE FOR CALCULATING KERMA AND DAMAGE
HEU	HIGHLY ENRICHED URANIUM
HLW	HIGH LEVEL WASTE
HPC	HIGH PERFORMANCE COMPUTING
IEU	INTERMEDIATELY ENRICHED URANIUM
IHECSBE	INTERNATIONAL HANDBOOK OF EVALUATED CRITICALITY SAFETY BENCHMARK EXPERIMENTS
INL	IDAHO NATIONAL LABORATORY
K	KELVIN
KCODE	MCNP MODULE FOR CALCULATING CRITICALITY
K_{EFF}	EFFECTIVE NEUTRON MULTIPLICATION FACTOR
KERMA	KINETIC ENERGY RELEASED IN MATERIAL
LANL	LOS ALAMOS NATIONAL LABORATORY
LBTL	LOWER BOUND THRESHOLD LIMIT
LEU	LOW ENRICHED URANIUM
LFI	DOES THE MATERIAL FISSION: 0=NO, 1=YES
LLW	LOW LEVEL WASTE
LRP	RESONANCE PARAMETERS INCLUDED: -1=NO, 0=NO BUT YES IN MF2, 1=IN MF2 BUT ADD THEM INTO MF3, 2=IN MF2 BUT DON'T ADD THEM INTO MF3
MAT	MATERIAL

MCNP	MONTE CARLO N-PARTICLE TRANSPORT CODE
MET	METAL
MeV	MEGA ELECTRON VOLT
MODER	NJOY MODULE FOR ASCII TO/FROM BINARY CONVERSION
MAT	MATERIAL
MF	ENDF MATERIAL FILE
MPI	MESSAGE PASSING INTERFACE
MT	ENDF MATERIAL SECTION
MTHM	METRIC TON HEAVY METAL
NJOY	NUCLEAR DATA PROCESSING SYSTEM SOFTWARE
NNDC	NATIONAL NUCLEAR DATA CENTER
Np	NEPTUNIUM
NSUB	NUMERICAL SUBLIBRARY OF AN ENDF MAT FILE
ORNL	OAK RIDGE NATIONAL LABORATORY
PENDF	POINTWISE EVALUATED NUCLEAR DATA FILES
Pu	PLUTONIUM
PWR	PRESSURIZED WATER REACTOR
QC	QUALITY CHECK/QUALITY CONTROL
PURR	NJOY MODULE FOR UNRESOLVED PROBABILITY TABLES
r	RADIUS
ROA	RANGE OF APPLICABILITY
ROP	RANGE OF PARAMETERS
RSICC	RADIATION SAFETY INFORMATION COMPUTATIONAL CENTER

SFR	SPENT FUEL ROD
SMF	SPECIAL METAL FAST
SNL	SANDIA NATIONAL LABORTORY
THERMR	NJOY MODULE FOR COMPUTING SCATTERING EFFECTS
U	URANIUM
UNF	USED NUCLEAR FUEL
UNLV	UNIVERSITY OF NEVADA AT LAS VEGAS
UNM	UNIVERSITY OF NEW MEXICO
UNRESR	NJOY MODULE FOR UNRESOLVED RESONANCE SELF SHIELDING
UREX	URANIUM EXTRACTION PROCESS
USL	UPPER SUBCRITICAL LIMIT
VIEWR	NJOY MODULE FOR CREATING POSTSCRIPT FILES
XS	CROSS-SECTION
XSDIR	MCNP CROSS SECTION DIRECTORY FILE
YMP	YUCCA MOUNTAIN PROJECT

CHAPTER 1: INTRODUCTION

Nuclear engineering is a profession with many duties. An example of one of them is for the process of designing, operating and maintaining nuclear reactors, [1]. Shielding and radiation decay knowledge is another strong area for this degree. One of the main tenants for being a nuclear engineer is having an in-depth understanding of the neutron life cycle and all the associated parameters and equations that involve neutron cross-sections.

The neutron is a building block of the nucleus for all matter. It stabilizes the nucleus so that additional protons can be combined and make higher numbered elements. This is possible through the use of strong and weak nuclear forces.

The neutron has about a 10-minute half-life, [2], and then decays into a beta particle (β), a neutrino (ν), and a proton. This process allows unstable isotopes to stabilize or at least be on a path to a stable isotope. The neutron decay process is also important for students studying astrophysics.

The neutron's life-cycle is quantified by the "Six-Factor Formula," [3]. It is the neutron life-cycle balance equation, which includes six separate factors, the product of which is equal to the ratio of the number of neutrons in any generation to that of the previous one; this parameter is called the effective multiplication factor (k), or K_{eff} . The term K_{eff} (real not ideal) can also be determined by $K_{eff} = L_f \rho L_{th} f \eta \epsilon$, where:

K_{eff} = neutron production from fission in one generation / (neutron absorption in the preceding generation + neutron leakage in the preceding generation)

L_f = fast non-leakage factor, the number of fast neutrons that do not leak from reactor/number of fast neutrons produced by all fissions

ρ = resonance escape probability, number of neutrons that reach thermal energy/number of fast neutrons that start to slow down

L_{th} = thermal non-leakage factor, the number of thermal neutrons that do not leak from reactor/number of neutrons that reach thermal energies

f = thermal fuel utilization factor, number of neutron absorbed in the fuel/number of neutrons absorbed in all reactor material

$$f = (\Sigma^U * \phi^U * V^U) / (\Sigma^U * \phi^U * V^U + \Sigma^M * \phi^M * V^M + \Sigma^P * \phi^P * V^P)$$

η = reproduction factor,

$$\eta = (\Sigma_f^U * \phi^U * \nu) / (\Sigma_a^U * \phi^U)$$

ϵ = fast-fission factor, is the number of fast neutrons produced by all fissions/the number of fast neutrons produced by thermal fission.

The six factor formula is an excellent tool for diagnostics. It is not to be used for design, because it needs input for the neutron flux from deterministic or transport codes. This is also an averaged or effective equation, not an exact one. This is because the cross-sections for the poisons, fuel, moderator and reactor vessel is smeared homogenously to simplify the formula. The equation will not provide exact solutions at any place in the reactor or experiment.

The superscripts U, M, and P refer to uranium, moderator, and poison, respectively. All of these equations involve using the averaged macroscopic cross-section, which is

$\Sigma = N * \sigma$. The macroscopic cross-section Σ is equal to the number of the material (N) times the microscopic cross-section (σ) of that material, [4]. This is important to understand, because this research paper addresses the status of the microscopic cross-section data, directly taken from Brookhaven National Lab's ENDF files. All equations that require " σ ," use the data from the ENDF files.

The neutron life-cycle and cross-sections are closely related in that as the neutron goes through the cycle from emission to absorption or decay, [5], it will change its energy level or speed. This in turn will change the probability of the surrounding materials to scatter or absorb the neutron. The affinity or probability of the isotope to scatter or absorb the neutron is measured by its microscopic cross-section. This is determined by the material bombarded by a neutron flux and having the experiment well-documented to calculate the probability of the isotope's reaction to the neutrons at varying energy levels. Cross-sections for a given material and neutron energy level change with the material's temperature as well, but that is outside the scope of this research. This data is then visually displayed by a graph of neutron energy level (MeV) vs. isotope cross-section (barns or cm^2). Think of a cross-section as a 2D/circular/target area or "bullseye", but measured in cm^2 , [6].

There are two basic forms of cross-sections: scattering and absorption. Scattering can be elastic or inelastic, while absorption leads to capture/activation or fission. These cross-sections are unique for each isotope for each element, as determined by the speed of the incoming neutron, [7].

This is important to understand that the neutron will have different behaviors at different energies through its life-cycle for the same material. Every material has its own unique set of cross-sections for the varying energies. So as the neutron progresses through its' life-cycle, the neutron will typically reduce in energy (speed) and either bounce around the material (scatter), escape the material (leak), or be absorbed into the material, [8]. Trying to exactly calculate this behavior is why we require calculation codes and nuclear data with the smallest amounts of uncertainties.

There are a few regions and items on a typical cross-section plot that is of interest, see

Figures 8-11. Cross-sections are divided up into areas by energy ranges. Going from left to right on the plot, the first area is the energy range from 0.0 to .025 eV, and it is for cold neutrons. This range is for neutrons that are slower than 2200 m/s.

The next range to the right is the thermal energy neutrons around 0.025 eV. These are the target neutrons that are required for PWR and BWR reactors to operate, due to the U-235 fuel. The cross-sections for U-235 is best for thermal neutrons. These are the neutron that are at 2200 m/s at 298K.

Epithermal energy neutrons are from around 0.025 eV to about 1eV. This energy range covers the area that includes the capture energy for the control rods made of cadmium. This is the energy range also that demonstrates the $1/v$ slope for energy to cross-section relationship.

The resolved resonance energy range will be from about 1eV (or 1.0×10^{-6} MeV) to about 0.5 MeV. This is where experimental data and complex computations have mapped out all the data points to define the peaks and valleys. The unresolved resonance range is from about 0.5 MeV to about 1.0 MeV. This is where the resonance peaks have yet to be determined.

Energies above 1.0 MeV are fast neutrons and these cross-sections approach the hard sphere diameter approximations. This means that the effective cross-section of a fast neutron will be approximately the cross-sectional or frontal area of the nucleus.

The American National Standards Institute publication for “Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors,” ANSI/ANS-8.1-2014, allows the use of calculations, in the form of accepted codes, in the determination of subcritical limits for the design of fissionable material systems, [9]. This process is applicable for fuel rod manufacturing, criticality safety benchmark experiments, as well as spent fuel rod shipping casks. This standard requires validation of the analytical methods and data used in the criticality safety calculations in

order to quantify any computational bias and the sensitivity in the bias. The NRC guidance requires ANSI/ANS-9.1-1998 be used but additional documentation for calculations and methods for conclusions are required, [10].

The historical validation process has been conducted by comparing the closest experimental results with the calculated results. The experimental results are well documented in the International Handbook of Evaluated Criticality Safety Benchmark Experiments, [11]. As many as possible parameters of the experimental and calculated projects must match in order to make the comparison as close as possible. Because the calculated and experimental projects may not be exactly the same, the engineer must assign an administrative bias to the calculations, indicating that the two do not exactly match.

The nuclear data has been attributed with inducing an additional small amount of bias, sometimes up to one percent [12]. This method allows the calculations to be quantified without having to construct and conduct an exact experiment. When the two results do not match, this has typically resulted in changing the codes to make the algorithms of the computed results closely match the experimental results, because the nuclear data has been taken as unchangeable.

When sensitivity and uncertainty (S/U) are talked about, they normally refer to calculations and work conducted concerning the classical perturbation theory and cross-section sensitivity data, [13]. This method allows the reader to understand the basic boundary conditions placed on the topic, and how the results are garnered. S/U is a broad topic and can involve numerous inputs, too many to be dealt with for this dissertation, but sensitivity will be specifically addressed, due to the nature of this paper.

Extensive computational work has been conducted in the area of S/U in the last decade or so demonstrating the validity/verification (V&V) and robustness of computational codes and

nuclear data for criticality safety, [14]. The ALICE code was the first of the codes that conducted resonance range calculations. The second code was created and used at Brookhaven National Laboratory and it was called EMPIRE. GNASH is the third major cross-section code, and the output is matched with experimental data for validation. The combination of these codes and experimental data is how improvements to the ENDF file formats are published. Currently, the ENDF/B format is on edition 7.1.

Some of the issues with conducting cross-section work is the discovery of how much is not known. It came to light to the ANS Cross-Section Working Group that only about 15 isotopes have high fidelity cross-sections through the entire range of energies. This is to include the higher energies, where fast reactors operate, because fast reactor research is the new item.

Because computational capability has improved greatly over the last decade, there are several methodologies that take advantage of this resource. They are usually typically associated with this type of computational work: integral parameter applications, uncertainty analysis theory, and General linear-least squares methods. All three of these methods require energy-dependent sensitivity profiles for multiple nuclides and reactions. This data is then utilized to calculate the relative difference in K_{eff} due to the perturbations in the cross-sections.

Sensitivity is denoted as measuring the delta in the change in K_{eff} , divided by the change in the change in average and overall macroscopic cross-section. This becomes a generalization of the cross-sections and the material in order to calculate the sensitivity, [15].

$$S_x = (\Delta K_{eff} / K_{eff}) / (\Delta \Sigma_x / \Sigma_x)$$

Uncertainty is analyzed in SCALE by the TSUNAMI module, by using the General Linear-Least Squares Methods (GLLSM). This is accomplished with input parameters from the sensitivity calculations (S_x) and covariance data created from generalized group-wise cross-

section data embedded in SCALE, [16]. The main issue of using this data is that most of the cross-sections are not detailed enough to provide small uncertainties. There are gaps where extrapolation is used to provide a basically complete cross-section, [17]. This induces a sensitivity from the processing code (NJOY) and older cross-section files. Directly dealing with the newest raw cross-section data from ENDF/B is better. Obtaining more detailed raw data from experiments is best, but this requires additional research funds.

Now that a basic understanding of S/U work is delineated, the area of concentration for this dissertation is specifically concentrated on the cross-section data itself. This is to analyze the effect that the cross-section data has on the computational codes and the S/U analysis for nuclear models. If this basic building block of the nuclear engineering world is off, then the differences will be amplified through all the calculations.

The scientific community has been making observations of reality and postulating them into data and equations for centuries. This is the typical method for developing the information needed to make the next step of understanding and comprehension in a field of study. For example, the sun and stars were observed for centuries until a rudimentary understanding of their cycles allowed mankind to begin navigation. So it is the same with nuclear engineering, the observations of the affinity for a neutron to interact with a nucleus must be observed and recorded numerous times before an approximation can be determined, [18]. The higher the number of observations (or N), the higher the accuracy is derived for the approximation, due to error is equal to the reciprocal of the square root of the sample size N , using Poisson distribution statistics.

Understanding that increased sampling improves the accuracy of the error leads us to the process of how to obtain better observations for the isotopic neutron cross-section data. This

process requires that the isotope be as pure as possible. This is to prevent contamination and overshadowing of the sampled isotope from another isotope. The impurity isotope can mask the sampled isotope. This is the case with U-235 and U-238, in the fast and resonance ranges. Unfortunately, the smallest amount of one isotope can easily mask or give exaggerated cross-sections for the isotope under review.

The cost to completely purify any element to a single isotope is almost prohibitively expensive. If it is for research purposes alone, the funding is difficult to obtain. A perfect example of this is the removal of U-238 from U-235 for reactor and weapons manufacturing, [1]. Reactor grade U-235 enrichment is typically increasing the percentage of U-235 from 0.71 to about 6 percent. This requires usually less than ten passes through the centrifuge process. Weapons grade U-235 requires increasing the enrichment from the nominal 6% to usually greater than 90 percent. This will require greater than 20 passes thru the same centrifuge process, [1]. In order to completely purify the U-235 to 99+%, would require a logarithmic jump in passes to remove the U-234 and U-238. As a result, the cross-sections of U-235 and U-238 have small impurities of the other isotope folded into their respective cross-section observations.

Another issue that has limited the cross-section research is the computing power required to calculate the cross-sections, once the sampling experiments were completed. This type of complicated computational capability was not readily available from the 1940s through the 1980s, when a large amount of cross-section experiments was conducted, [19]. This produced numerous cross-sections that were incomplete or has a large sensitivity. The simple unfolding that was required to produce the neutron cross-sections, was available but they were only available for limited energy ranges, [19]. Currently, numerous neutronics codes can operate on a modern laptop or tablet, thus demonstrating the improved computational capabilities of

electronics. NJOY, MCNP, and SCALE are all perfect examples of this improvement.

In the past, the numerous cross-section experiments have produced many data points for U-234, U-235, and U-238. The problem is that the data points have “blank space” in between the points, and these gaps required interpolation by the codes that employ the cross-sections, [20]. There is significant concern from the scientific and commercial industries about the sparseness of the measured data, thus requiring a high sensitivity. This high sensitivity induces a large safety margin, which will then become a decrease in operational performance in the design. This can translate to millions of dollars wasted if it is in “overly” safe shipping casks or “under-utilized” reactor design, [21]. Both of these topics rely on small uncertainties in the neutron cross-section data in order to calculate the optimal efficiencies for the best design.

Burn-up credits are another point of contention that is not allowed by the NRC. This is so that the fuel estimates for burial/storage are as conservative as possible. Because the exact neutron flux cannot be calculated for the entire spent fuel rod (radially and axially), fresh fuel estimates are required to be used in place of the spent fuel. While this is only a difference of 5% U-235, this greatly hampers the ability of the commercial to store more fuel in a fewer number of casks. This is to prevent criticality issues in the spent fuel cask in any possible contingency. Because the spent fuel is only at 1-1.5% U-235, more spent fuel rods can be possibly stored in the same size cask, thus saving the commercial industry millions of dollars, and decreasing the require repository space.

Because the computational power in the 1940s through the 1970s was sparse, the data for criticality and neutron cross-sections had to be obtained physically through benchmark criticality experiments. GODIVA, JEMIMA, GODIVER, FLATTOP, and others, formed the core of the criticality experiments. These experiments had exact parameters that allowed the physicists to

obtain the observed data and then calculate the estimated cross-sections.

Neutronic computer codes were developed to match experimental data and the calculated results, [22]. These codes were refined as additional experiments were conducted. The basis of these codes are the ENDF data that is embedded in the material libraries in the databases. Sandia, Los Alamos and Livermore all have their own material libraries. Each laboratory has its own way to group the energy bands of the cross-sections. This grouping uses averages over the energy band, removing any peaks or valleys. The lower the number of energy groups, the more the energy is averaged across a larger energy range. This leads to increased errors in the neutron computational codes. The higher the number of groups in the database library will provide a better representation of the exact cross sections for the isotope through the energy from fission to absorption.

The impact of improved cross-sections research can produce smaller uncertainties and better sensitivities, [23]. Improved cross-sections will produce more accurate calculations for reactor design and spent fuel storage casks. More accurate designs will allow smaller reactors and safer storage for the spent fuel. This can translate into a larger safety margin and possible higher storage capacity for the casks. This can save the commercial industry millions of dollars in casks and thousands of square feet in storage space in underground repositories. It can also produce smaller reactors requiring less fuel. Fast reactors can also be better designed with the refined cross-sections, thus assisting with supplying the electrical needs of the nation.

CHAPTER 2: REVIEW OF RELATED LITERATURE

From 1940 through the late 1950s, neutron cross-section research was not usually published for public release, [18]. The reasons were not specified, but it could have been due to lack of format and medium or to undocumented classification reasons. Post-WWII, the data was maintained by the U.S. AEC, in order to limit promulgation of information about the design of atomic weapons. There are very few documents from this time period about most of the cross-section experiments.

Because of the lack communications between the two the group that was making cross-sections and other group that was using cross-sections, the neutron cross-section determinations were uncoupled with actual cross-section usage, [24]. This lead to cross-section experiments that produced data that was not perfectly needed or completely useful to the cross-section usage group. This was not readily understood until stronger computing capabilities were used with the neutronic codes and the uncertainties were discovered to be larger than acceptable. This was too late to redo the experiments and include things like covariance data into the format.

Before high speed computers became readily available for criticality calculations, hand calculations were provided in order to determine a quick K_{eff} , [25]. These hand calculations use simple one-group/modified one-group diffusion theory and buckling conversion calculations for estimating the K_{eff} . The issue with these quick calculations was that a simple geometry and averaged cross-sections were used, and the result is not representative of any location or flux in the reactor or experiment. Accurate 3-D flux calculations are required before operations.

While diffusion theory is simple and has limitations, it can be close for determining a quick K_{eff} by hand, [25]. The issue with using this method is that the sensitivity is large for the

resultant answer. Sensitivity is definitely the “friction of war” in nuclear engineering calculations.

Experimental data provides the basis for the computational neutronic codes, that are used to determine the criticality of systems, [26]. Even when the experiment is exactly matched with the code, there is still a sensitivity that resides in the codes. This sensitivity must be accounted for when estimating the final K_{eff} . The reduction of this sensitivity is needed to improve the accuracy of the computation codes.

This reduction in sensitivity is accomplished by improving the computer codes and refining the cross-sections. It is estimated that a difference in 1% in K_{eff} is able to be equated to a difference in 3% of mass for a critical system, [26]. The lower the enrichment, the higher the mass difference will be. This can be correlated to the better that K_{eff} can be calculated, then the more accurate that critical mass can be determined for the experiment. Codes and cross-sections are the key to improving safety margins and increasing the system’s efficiency.

Errors in calculations can be propagated through a design, to the point that it is detrimental to the safety of the design. Case in point is when the MAPLE reactors in Canada were designed in the 1990s, they were supposed to have a negative reactivity coefficient of $-0.12 \delta k/MW$. When rod testing was conducted in Jun 2003, it was demonstrated to repeatedly be $+0.28 \delta k/MW$. This means that on an up-power excursion, the reactor would increase power rapidly and would not be inherently designed to be able to be shut down, even with rod insertion. This makes the reactor completely inoperable. These mistakes can be hard to find with errors carried forward through the design process.

Improvement of cross-section data will have a direct correlation on the improvement in the computational code output. Three codes in particular that will benefit greatly from this

improvement, are NJOY, MCNP6\X, and SCALE. These codes are used by the commercial nuclear world and government agencies. There are many others, but these are within the scope of this topic, and the three of the codes benefit for different reasons.

Cross-section data is obtained from the cross-section experiments conducted at the various DoE labs. It is formatted, under the heading of ENDF data files, [27]. When additional experiments add further detailed data points, the overall ENDF file data for that isotope is improved. The ENDF files are then formatted into usable cross-section files in ACE formats, by a code called NJOY. The NJOY software then arranges and formats the data to be in the correct sequence for various codes. Two of the popularly mentioned neutronics codes are SCALE and MCNP6\X.

Understanding the structure of the ENDF files is extremely important in targeting the research to help improve the overall data file content. This focused research is able to be applied to a wide variety of new applications covering advanced reactor design, nuclear waste transmutation, fusion, medical applications space physics, and homeland security, [28].

Comprehension of the structure of the ENDF file format is required to be able to apply the appropriate research into the correct subparts for an improvement in the overall data files. The ENDF file format is an evolving process, [27], and has changed several times. This is in response to the demand from the cross-section users to include additional data that was previously overlooked. Covariance data (NSUB 19) is a perfect example of this inclusion of information into the current format.

The ENDF file format begins with the ENDF Library number (NLIB). This number uniquely identifies from where the data originated, [27]. The below Table 1 lists a few of the top NLIBs that are commonly used in ENDF file formats.

Table 1: NLIB Numbers

1	ENDF/B-VII.1 (USA, 2011)
2	JEFF-3.2 (Europe, 2014)
3	JENDL-4.0u2 (Japan, 2012)
4	CENDL-3.1 (China, 2009)
5	ROSFORND-2010 (Russia, 2010)
6	BROND-2.2 (Russia, 1992)

The next identification for a ENDF file will be the MAT number. This number identifies a specific isotope. The isotopes of concern for this topic are U-234/9225, U-235/9227, U-236/9231, and U-238/9237.

The next subdivision for the ENDF file formatting is called NSUB, [27]. The NSUB is about the induced or incident particle data. Table 2 lists some of the important NSUB libraries.

Table 2: NSUB-library Numbers and Names

0	Photonuclear data
1	Photo-Induced Fission Product Yields
3	Photo-Atomic Interaction Data
4	Radioactive Decay Data
5	Spontaneous Fission Product Yields
6	Atomic Relaxation Data
10	Incident-Neutron Data
11	Neutron-Induced Fission Product Yields
12	Thermal Neutron Scattering Data
19	Covariance Data

The above table is a small representation of the NSUB libraries. Many of the NSUB libraries do not pertain to this topic, so they are not included in the discussion or research. To

keep the scope of this dissertation within reason, only the NSUB 10 library will be considered. This is due to the other NSUBs not containing cross-section data. This is to focus the scope of the research to incident neutron cross-sections that cause fission.

Each NSUB is then further subdivided up into Material Files, identified by a MF number. Each MF number contains the data for a certain class of information for that specific isotope only. MF sections comprise specific data for the MAT being analyzed. Table 3 lists some of the important MF sections.

Table 3: Material File (MF) Numbers and Names

1	General information
2	Resonance parameter data
3	Reaction cross sections
4	Angular distributions for emitted particles
5	Energy distributions for emitted particles
6	Energy-angle distributions for emitted particles
7	Thermal neutron scattering law data
8	Radioactivity and fission-product yield data
9	Multiplicities for radioactive nuclide production
10	Cross sections for radioactive nuclide production
12	Multiplicities for photon production
13	Cross sections for photon production
14	Angular distributions for photon production
15	Energy distributions for photon production
23	Photo- or electro-atomic interaction cross sections
26	Electro-atomic angle and energy distribution
27	Atomic form factors or scattering functions for photo-atomic interactions
28	Atomic relaxation data
30	Data covariances obtained from parameter covariances and sensitivities
31	Data covariances for $\nu(\bar{\nu})$
32	Data covariances for resonance parameters
33	Data covariances for reaction cross sections
34	Data covariances for angular distributions
35	Data covariances for energy distributions
39	Data covariances for radionuclide production yields
40	Data covariances for radionuclide production cross sections

MF sections contain more than just cross-section data. Some MF sections contain text only (MT1) or energy bands (MT4-6) for specific angles of incidence. To keep the boundaries and scope of this dissertation within reason, only the sections of MF3 will be considered. This section of the ENDF file format is the only section that affects the cross-sections for scattering and fission.

Continuing deeper into the ENDF file tape, the MF is then continued to be divided up into more subdivisions, each one containing data for a particular reaction type, identified as a MT number). The MT is a specific reaction with specific parameters for the target material. Table 4 lists some of the important MT sections out of the MF sections.

Table 4: Material Type (MT) Numbers, Reactions, and Names

1	(n,total)	Neutron total cross sections. Sum of MT1=MT2+MT3
2		Elastic scattering cross section for incident particles.
3		Non-elastic neutron cross section
4	(z,n)	Production of 1 neutron in exit ch. Sum of MT=MT50+MT51...MT91
5		Sum of all reactions not given in another MT, added to MT1
18	(z,fission)	Particle-induced fission. Sum of MT18= MT19+MT20+MT21+MT38
19	(n,f)	First-chance neutron-induced fission
20	(n,nf)	Second-chance neutron-induced fission
21	(n,2nf)	Third-chance neutron-induced fission
38	(n,3nf)	Fourth-chance fission cross section.
50-	(y,n)	Production of a neutron, leaving the residual nucleus in ground state
102	(z, γ)	Radiative capture.

The MT of importance for this research is MT1, MT4, and MT18, and the parts that make up the sums of each of those MTs. While the other MTs are important in reactions with the materials, the data required as input for NJOY does not include MT sections outside of those two in order to calculate the cross-sections.

Finally, a Material Type is divided into Material Records or MR. These are the individual observations from specific experiments, or combination of experiments, to obtain the data or

cross-sections. Individual MRs will not be directly referenced, but the summation of their inputs assist in forming the entire MT file. This is the level of data that will be perturbed by the Fortran code.

A comparison of the ENDF files for the isotopes of concern: U-234, U-235, U-236, and U-238 are shown in Appendix A. This is attached to show the different content of the ENDF files for each isotope. Each MAT has different observations and characteristics; therefore, each isotope will have a different content of MTs.

Understanding the content in an ENDF file for a MAT/MF/MT section, requires the ability to directly read the ENDF file in its' native text format. The ENDF files can be downloaded from Brookhaven National Laboratory's Internet site under the keyword "ENDF." The file is then selected by MAT and NLIB desired. The file is in a readable text format and is formatted in 80 columns and divided by MT sections.

Figure 1: Example of ENDF File Formatting

```

Retrieved by E4-Web: 2015/12/15,13:52:37
9.223400+4 2.320304+2 1 0 0 0
0.000000+0 1.000000+0 0 0 0 0
1.000000+0 3.000000+7 1 0 10 0
0.000000+0 0.000000+0 0 0 375 1349225
92-U -234 ORNL,LANL+ EVAL-APR06 Young,Kawano,Chadwick,MacFarlane 9225 1451 5
DIST-DEC06 REV2- 20111222 9225 1451 6
-----ENDF/B-VII.1 MATERIAL 9225 REVISION 2 9225 1451 7
-----INCIDENT NEUTRON DATA 9225 1451 8
-----ENDF-6 FORMAT 9225 1451 9
9225 1451 10
9225 1451 11
=====
Covariances - BNL, Oct, 2011: Covariances were adopted from 9225 1451 12
COMMARA-2.0, which were supplied by BNL. Covariances are a 9225 1451 13
combination of the uncertainties recommended in the assessment 9225 1451 14
of Ref. [1] and correlation matrices produced by the WPEC 9225 1451 15
Subgroup 26 [2] which were converted to the AFCI 33-energy group 9225 1451 16
structure. The initial estimates were obtained using EMPIRE/KALMAN 9225 1451 17
system with default parameterization roughly adjusted to 9225 1451 18
reproduce trends in the experimental data. The KALMAN code was 9225 1451 19
run with default uncertainties assigned to the key model 9225 1451 20
parameters to produce covariances. Following the low-fidelity 9225 1451 21
approach, the uncertainties in the low energy region are based on 9225 1451 22
experimental uncertainties of thermal cross sections, 9225 1451 23
uncertainties of the resonance integrals and uncertainty of the 9225 1451 24
scattering radius. The assessment of Ref. [1] set elastic 9225 1451 25
uncertainty at 4%, confirmed Subgroup 26 fission and (n,2n) 9225 1451 26
uncertainties, modified inelastic, an slightly increased 9225 1451 27
capture uncertainty. 9225 1451 28
9225 1451 29
[1] V.M. Maslov, P. Oblozinsky, M. Herman, "Review and Assessment 9225 1451 30
of Neutron Cross Section and Nu-bar Covariances for Advanced 9225 1451 31
Reactor Systems," Report BNL-81884-2008-IR, Brookhaven 9225 1451 32
National Laboratory (2008). 9225 1451 33
9225 1451 34
[2] D. Rochman, M. Herman, P. Oblozinsky, and S. F. Mughabghab, 9225 1451 35
"Preliminary Cross Section Covariances for WPEC Subgroup 26," 9225 1451 36
Report BNL-77407-2007-IR, Brookhaven National Laboratory (2007). 9225 1451 37
9225 1451 38

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In Figure 1, the column numbers are labeled at the top of the figure. The Columns 1 through 67 is the text or the specific data pertaining to that MT, Columns 68 through 70 is the MAT number, Columns 71 through 72 is the MF number, Columns 73 through 75 is the MT number, and Column 76 through 80 is the line number for the specific MT section, with 99999 indicating the end of the MT.

The data is written in Columns 1-67, and are in pairs of numbers. For the MF3 sections that are cross-sections, the pairs of numbers are written as energy (eV) – with an associated cross-section (barns). The energies and the cross-sections are written as a ten column scientific notation numbers with a space between the energy and the cross-section, as well as a space between the next pair. There are three pairs in a row from Column 1 through 67. The header information at the beginning of the MT will be three rows, and the header will state twice how many energy-cross section pairs there are documented in the MT file. Figure 2 shows an example of the first ten lines of MAT 9225/MF3/MT1, including the header and first seven rows of data pairs.

Figure 2: ENDF File Data Contents

9.223400+4	2.320304+2	0	0	0	09225 3	1	1
0.000000+0	0.000000+0	0	0	1	4399225 3	1	2
439	2				9225 3	1	3
1.000000-5	0.000000+0	1.500000+3	0.000000+0	4.368748+4	0.000000+09225 3	1	4
5.000000+4	6.699730-2	6.000000+4	1.635648-1	7.000000+4	2.497003-19225 3	1	5
8.000000+4	3.261182-1	9.000000+4	3.935892-1	1.000000+5	4.528497-19225 3	1	6
1.000000+5	1.195876+1	1.100000+5	1.182126+1	1.200000+5	1.168775+19225 3	1	7
1.300000+5	1.155858+1	1.400000+5	1.143406+1	1.439176+5	1.138663+19225 3	1	8
1.500000+5	1.131455+1	1.600000+5	1.119819+1	1.700000+5	1.108338+19225 3	1	9
1.800000+5	1.097086+1	1.900000+5	1.086135+1	2.000000+5	1.075556+19225 3	1	10

Now with a basic understanding of ENDF file formatting, the area of detailed focus will

be the MAT/NSUB10/MF3/MT (1, 4, and 18) sections for all four isotopes. MT 1 will include MT2, and MT3, while MT18 will include MT19, MT20, MT21, and MT38. Resonance regions (MF2) improvements are very important, and can be documented better with more cross-section experiments, but that analysis is a follow-on topic for other research efforts. The changes in the sensitivity of the cross-sections are the focus for this dissertation.

Table 5: Modules of NJOY

RECONR	Reconstruct point-wise cross-sections
BROADR	Doppler broadens and thins neutron point-wise cross-sections
UNRESR	Calculates Self-shielded, unresolved resonance cross-sections
HEATR	Computes kinetic energy deposited and radiation damage in material
THERMR	Generates scattering cross-sections & point to point scattering kernels
GROUPE	Produce self-shielded XS, neutron scattering and photon production matrices, then to MATXS module
GAMINR	Calculates multi-group photo-atomic XS, kerma factors, and Group to Group scattering matrices
ERRORR	Computes multi-group covariance matrices, and then to COVR module
COVR	Reads ERRORR output and performs covariance plotting and output
MODER	Converts ENDF tapes back and forth between ASCII and binary
DTFR	Formats multi-group data for transport codes like DTFR-IV
CCCCR	Format multi-group data for ISOTXS, BRKOXS, DLAYXS codes
MATXS	Formats multi-group data for MATXS, works with TRANSXS
RESXS	Prepares point-wise XS in CCCC form
ACER	Prepares libraries in ACE format for LANL MCNP6\X codes
POWER	Not used
WIMSR	Not used
PLOTR	Makes XS plots and plots views for both point-wise and multi-group XS
MIXR	Used to combine XS into elements or mixtures, mainly for plotting
PURR	Used to prepare unresolved region probability tables for MCNP6\X codes

The first professional code to be discussed is NJOY. It is a LANL code that uses the input of the ENDF data files from numerous cross-section experiments and arranges the cross-section data into the correct format for the computational code, [29]. The software takes specified sections of the raw data files from the ENDF format and arranges them into a readable format

(ACE) for the appropriate neutronics code. When compiling the new cross-sections, the code fails and reports to the user of the MF or MT sections that are missing. This is why it is important to understand the structure of the ENDF library.

NJOY is a FORTRAN based code that is updated and compiled by the end user. The code is comprised of 20 modules. The main NJOY code is ran with an input file that instructs the code which module to use and where the raw ENDF files are located. The modules of NJOY are listed in Table 5.

The NJOY code is executed with a DOS batch file. This batch file lists the input ENDF files and the *.dat file, which lists the modules that will be used on the ENDF data. These modules must be arranged in the correct order or the NJOY program will fail. The output of one module feeds the input of the next module.

The key modules that are to be used to create the new cross-sections for the perturbation are: MODR, RECONR, BROADR, UNRESR, HEATR, THERMR, GROUPT, ACER, PURR, PLOTR, and MIXR. In Table 6 is a list of the sections of ENDF files that are needed for the modules to correctly compile the new XS, with the appropriate ENDF MT sections that will be required in the input ENDF files. If these sections are not in the ENDF file, the NJOY code will crash. This is why it is important to be able to read and understand the internals of the ENDF file format.

The MCNP6 and MCNPX (MCNP6\X) codes both use ENDF files, in order to calculate K_{eff} . SCALE is explained here to show comparative software to MCNP6\X, but it is not used in any of the calculations. It is a very important software in the nuclear engineering industry and will also reap benefits from improved cross-sections experimentations. Future thermal and fast reactor designs will benefit from these improvements to the cross-section data.

Table 6: Sections of ENDF Required for the Modules of NJOY

RECONR	MF1(MT451), MF2(MT151,152), MF3(MT1, MT2, MT18, MT102), MF10, MF13
BROADR	MF3(MT1, MT2, MT18, MT102)
UNRESR	MF2 (MT152), MF3(MT1, MT2, MT18, MT102)
HEATR	MF1(MT458), MF3 (MT1, MT2, MT18, MT102), MF4, MF5, MF6, MF12, MF13 (MT3, MT4), MF15
THERMR	MF1, MF3(MT1, MT2, MT18, MT102), MF6, MF7(MT2)
GROUPT	PENDF input and MF3(MT1, MT2, MT18, MT102), MF4, MF5, MF6, MF12, MF13, MF15, MF18,
MODER	Any and all MF/MT combinations
ACER	PENDF and GENDF, directly taken as input
PLOTR	Directly takes last module output as input
PURR	Directly takes last module output as input
VIEWR	Takes any PENDF or GENDF module as input

The two neutronic codes of interest use a processed version of the cross-sections from the raw data ENDF cross-section files. Each isotope file includes the capture, fission, elastic, and inelastic scattering cross-sections. Each of the different cross-sections are used for the appropriate reaction when evaluating the neutron for the life cycle in the code's equations. This is automatically accomplished by the SCALE and MCNP6\X software.

The SCALE code is used to produce analysis about reactor design and fuel rod burnup and decay. SCALE's criticality and depletion codes use the ENDF/B-VII cross-sections, [30]. This is possible after the cross-sections have been processed through a code called AMPX, which is like NJOY.

The criticality module of SCALE is called KENO. Criticality calculations are conducted with either the KENO-Va or VI modules. Both versions can do 3D analysis, but the VI version can utilize simple geometric patterns and build complex models from those simple patterns. If a fast model is need, then only use KENO-Va.

Since cross-sections are the focal point of this dissertation, it is only fair to discuss some of the issues about them, as dealt with in the internals of the neutronics codes. As previously mentioned, two requirements are needed for the neutronics codes to properly process data, and those are neutron energy and the associative cross-section. This can be represented two different ways, either by a continuous energy curve or by dividing up the continuous energy into energy groups.

A continuous energy group is represented by all the energy points for the neutron covering the entire cross-section curve. This curve is the most accurate because all data points are included. The drawback to using a continuous energy curve is that the process greatly increases the computing time, because every point is evaluated along the continuous energy curve.

A group-energy curve is made from the same continuous energy points, but the curve is divided up into sections and those sections are spectrum energy averaged. The data points in those sections need to be relatively close to each other, or large uncertainties will be introduced into that energy group. For example, the LANL 44-group set of cross-sections, divided up the energy versus cross-section curve into only 44 sections for an energy range of 2.5×10^{-2} eV to 20 MeV. The ORNL 238-group subdivides the curve six more times, giving it a more refined set of groupings.

If faster calculation times are needed, then replacing the continuous neutron energy cross-sections with a 238-energy group cross-section neutron library will produce faster run times. This simplifies the calculations for SCALE, yet some definition is lost in the cross-section analysis when this occurs. In comparison, the depletion module SAS2H/ARP/ORIGEN-SCSASI/WAX uses the 44-energy group cross-section gamma library because depletion does not

require detailed energy curves.

The unprocessed ENDF data needs to have the smallest amount of inherent sensitivity, so that the errors are not increased as they are propagated through the calculations. Using the current SCALE code, with the associated AMPX generated SCALE cross-sections for a high capacity rail cask, the code can calculate differences in K_{eff} varying from 0.02 to 0.05. This is due to a single SNF assembly misload, [30]. This amount of propagated sensitivity is why it is important to have the neutron cross-sections need to be as accurate as possible.

For the NRC, the actual SFR cask or repository storage is conducted by using the “fresh fuel” or un-irradiated fuel concept, [31], due to the concept that the sensitivity for the codes and cross-section data is too large to be accurate enough for actual historical representation of the true burnup of that fuel rod. Due to the limited accuracy for some of the fission yield products, this provides no allowances to the reduction of reactivity nor the increase of neutron poisons due to burnup of the U-235, [32]. This results in a higher K_{eff} in the cask or repository storage calculations due to all the fresh fuel, which is truly not present in a SFR. This is a compound issue if the cross-section sensitivity is already large.

Current estimates of burnup, that include in-core instrumentation, are within 2% of values produced from design codes, [31]. When conducting zero-power physics testing (ZPPT), up to about 5% burnup error can be missed due to instrumentation limitations, [31]. Better instrumentation and neutron codes, with reduced cross-section sensitivity, can decrease this error between the burnup errors and core loading in the neutronics codes, SCALE in particular. This error will be summed with the already present sensitivities.

Providing SCALE with improved cross-sections will improve the burnup credits as calculated from the depletion modules. With the improved cross-sections to match current and

future experiments, the commercial industry will be able to more accurately calculate the burnup for the commercial nuclear power plants (NPP) and SFR repositories, thus providing more accurate data for the true burnup in each SFR. This will greatly increase the cask capacities for the same given cask designs, possibly from 24 to 32, [33]. This increase in cask storage will produce increased cost savings and reduce storage area by up to 30%. This also means a reduction in long term storage area required for the casks, [33].

TSUNAMI is another module in SCALE. It is used to calculate uncertainties and covariances for the desired cross-sections. TSUNAMI's validation techniques for uncertainties deal primarily with computational biases that are caused by errors in the nuclear cross-section data [12]. These are quantified in the cross-section-covariance data contained in the isotope's ENDF file sections MT31 and MT33. The problem with the covariance data is that it is only estimates, not actual data. This can lead designers astray if they are relying on the two sections of the ENDF file to be highly accurate.

The MCNP code is one of the other major pieces of software that will be discussed. It is a mature mathematical neutronics code used by labs and academic personnel, that uses a stochastic method for determining the neutron flux, [34]. It uses the Monte Carlo principle as the main method for the neutron transport calculations. The results of a Monte Carlo run are very close to an answer from the Boltzmann equation, in integral form. This is a powerful tool, without requiring seven variables to be solved simultaneously.

MCNP6 and MCNPX are the two flavors of the code from LANL. MCNP6 is the standard because it is robust and has years of V&V certification. MCNPX is more versatile because it can calculate the transport of subatomic particles to heavy ions through most materials. Monte Carlo is the microscopic way of calculating neutron transport, because every

neutron's path is individually calculated.

MCNP6\X, an acronym meaning both MCNP6 and MCNPX, are codes written in Fortran 90 and requires rigorously formatted text files as input statements. Deviation by even a misplaced space or tab will render the entire input as useless. It can build complex geometries just like KENO.

MCNP6\X is also multicore capable. Using MPI or HPC software, all available cores on a computer can be used for the calculations. Most software codes can only utilize one CPU at a time. This greatly speeds up the time required to calculate a problem set.

MCNP6\X's calculation method uses the ENDF nuclear data libraries that are characterized by a continuous-energy representation. This library of cross-sections is created by NJOY and is Type I ACE formatted. The code output is based on a very fine energy resolution of the cross-section's energy dependence. MCNP6\X may require long calculation times in order to ensure that total energy deposition is appropriately captured into the material from the interacting particle(s).

In MCNP6\X, the particle being tracked is a neutron, and the interacting material is a fissile isotope, this is the perfect situation for MCNP6\X to be able to conduct criticality calculations, and thus to determine the overall K_{eff} , [35]. This is neutronic code is generally far easier to use and more flexible than KENO, and uses an external software program called Visual Editor (VizEd) to assist in creation of the input files. KENO uses GeeWiz as a GUI for creating the input decks for SCALE.

A basic MCNP6\X input deck is divided into three sections. All lines must end at the 80 column mark, or a fatal Fortran error will occur. Traditionally, eight sets of "0123456789" are strung together as the first row of the deck, to delineate the max width of all following lines.

Anything that is greater than the 80th column is ignored by the program, but if the extra code is necessary as program input, then a crash will occur. If tabs are used as spaces, the code will crash as well.

The first section contains few rows are identifying rows for the title, author, and scope of the deck. These lines are prefaced with the letter C, for continue, or pass over. This directs the program not to execute or count this line as code. You can have as many C lines as you need, to help instruct the reader, not the program, on what and why and how you are making your model. The second part of the first section is separated from the title section by a blank return line. The next lines are called cell cards. They are the objects of the model, made of the shapes in the second section. Each cell card has the density, bounding surfaces and particle weights per cell. Various combinations of surfaces from the second section of the deck can make a cell card.

The second section is purely the construction of the surface cards. Each object created in the first section of the input deck must be clearly defined by surfaces in the second section. MCNP6\X has numerous macro-bodies that are understood by the code as surfaces; and that allows easier construction of cell cards.

The third section has the material cards and data cards. The material cards are the ACE formatted cross-section libraries, located in the “MCNP_DATA” directory. This is where the newly perturbed cross-sections will be substituted. The data cards are the program definitions that instruct the code on what to execute, with the materials, surface and cell cards.

The resulting output file requires understanding of the input file and an understanding of the definitions of the construction of MCNP6\X to be fully comprehended. MCNP6\X is not a black box, [34]. It is a robust and capable tool for criticality and shielding calculations.

MCNP6\X will also be used to validate the perturbed cross-sections by calculating the

two Criticality Benchmark Experiments HMF-001 and HMF004. The new results will be compared with the documented results from the IHCSBE handbook. Many of the Criticality Benchmark Experiments provide a SCALE/KENO and MCNP6\P input, [11], in the write-up of the experiment.

Both of these software codes MCNP6\X and KENO are stochastic in how they determine K_{eff} . These codes are stochastic processed where the input is randomized, and is calculated by observing the behavior of the particle on an individual basis, in order to calculate K_{eff} . This provides a microscopic view of the inputs to the mathematical process.

In comparison, a deterministic code is where the neutron flux is calculated directly by using the neutron transport integral differential equations (Boltzmann), [36]. This provides a steady method for the mathematical process and is a macroscopic view of how to macroscopically calculate K_{eff} . The problem with this mathematical method is that it is slow and iterative process, and many of the physics are hidden in the scattering kernel and cross-sections.

The calculated results are then compared and matched with actual experimental data K_{eff} in the IHECSBE. The difference between the calculated and the experimental results is usually only a hundredths of a decimal place. This provides excellent reliability to validate the neutronics codes when actual experimental data is unavailable.

Both of the neutronics codes are only a few hundredths of a decimal place different from each other for the K_{eff} , as well as versus the actual experimental data. This allows a high level of confidence by the users when creating new models. Unfortunately, confidence does not translate into usable numbers that are defensible for creating a sensitivity policy or doctrine.

One of the main documents for referencing the two key benchmarks experiments of this dissertation, HMF-001 and HMF-004, is the International Handbook of Evaluated Criticality

Safety Benchmark Experiments, [11]. This reference comes in CD format from the Idaho National Laboratory. The evaluated experiments in the IHECSBE are presented as simple geometric models. Minimizing the details of the models allows the KENO and MCNP6\X software to run as efficiently and quickly as possible.

By selecting the two experiments, HMF-001 and HMF-004, the analysis is localized to only four uranium isotopes. These are U-234, U-235, U-236, and U-238. This places boundary conditions how many isotopes require use of the Fortran-made perturbation software.

HMF-001 and HMF-004 also have different neutron energy spectra. This ensures that the perturbations can be applied to two experiments with similar geometries yet dissimilar environments.

Recent re-evaluations of criticality benchmark experiments, specifically concerning the bare HEU sphere, unreflected and water-reflected, have revealed that the neutron spectrum softened more than previously noted, [37]. As the cross-sections for U-235 are further refined, it has shown a trend for the K_{eff} to decrease, while the U-238 cross-section evaluations have caused K_{eff} to increase. This analysis shows that the Energy/Cross-section curve for U-235 has decreased overall, while the U-238 one has increased. This is also very dependent on the experiments' neutron energy spectrum and ratio of U-235/U-238. This softening of the neutron spectrum in HMF-004 allowed a similar comparison against HMF-001.

Selecting the appropriate model for perturbing the cross-sections came down to possible five possible models. The selection criteria were as follows: simple model, minimal isotopes, experimental data is available, and finally must have been modeled in MCNP. After researching several publications, the two models, HMF-001 and HMF-004, provided excellent results to the boundary conditions, [38].

Neutron spectrum is also an important measure for criticality benchmarks, [39]. The objective is to compare two “like” spectrums. Having the models just slightly different, will allow close comparisons, but also demonstrate that small changes in the models will appropriately change the spectrums. A fast or hard spectrum is easier to compare, due to simplicity of the curve displaying the neutron distribution in the high energy ranges.

The sensitivity of the cross-sections is formative in determining the biases for documented experiments, [9]. The bias sensitivity is based on the environment and the controlling factors of the experiment. The larger the sensitivity is for the factors, the larger the bias is to be, which will administratively limit the maximum K_{eff} allowed for the experiment. This is to provide a safety margin on the K_{eff} value, in order to prevent accidental criticality. The smaller the sensitivity in the factors, including the contributing cross-sections, the smaller the bias, and the smaller the administrative bias will be for the estimated K_{eff} .

How does sensitivity and uncertainty effect the calculations for the two experiments HMF-001 and HMF-004? Sensitivity is the measure of change in K_{eff} when changing a control variable, [23]. The following equation denotes that for the forward form of the neutron transport equation: $A\phi=1/k (B\phi)$, where:

$k = K_{eff}$, the neutron multiplication factor,

A = an operator that represents all of the transport equation, except for the fission term,

B = an operator that represents the fission term in the transport equation.

ϕ = multigroup adjoint flux, composed of different spatial and energy groups.

The ability to perturbate the various constants in the neutron transport equation allows the effect of K_{eff} to be determined, except for being able to vary the cross-sections themselves, [40].

The sensitivity of the variable directly proportional to the percent change in the K_{eff} , [40].

Uncertainty is determined by calculating the relative multi-group, covariances matrices for the two reactions. The two reactions can be same-type or dissimilar reactions. If the reactions are in dissimilar energy groups or different zones of the experiment, then the coefficients are summed, [40]. Unfortunately, the summation can give rise to an inaccuracy because resonance-shielded cross sections that vary by zone are used to calculate the zone-wise sensitivity coefficients; and the cross-section covariance files are for infinite-dilute cross-sections. This treatment assumes that the relative uncertainties of shielded cross sections are similar to the relative uncertainties of unshielded cross sections.

$$\sigma^2 = \sum_{x,y,g,g'} [S_{g,x} \text{Cov}(x_g, y_{g'}) S_{g',y}], \text{ where}$$

$$\text{Cov}(x_g, y_{g'}) = \frac{\langle x_g - x_{g_{ave}} \rangle \langle y_{g'} - y_{g_{ave}} \rangle}{x_{g_{ave}} y_{g_{ave}}}$$

Efforts have been made to improve the overall quality of the nuclear data available for neutronics codes, [41]. Reactor designs and other applications have been the driving force for new data evaluations in the low energy range. Evaluating the neutrons in the high energy region have been accomplished primarily in support of shielding applications and fast reactor design. Although the accuracy of the nuclear data, such as the cross sections, has improved, more research is still need on nuclear data uncertainties, (i.e., nuclear data covariance). The uncertainty files in the ENDF/B library are obtained from analyses of experimental data and are stored as covariance and sensitivity data.

The problem with using the current cross-section ENDF/B files is that the uncertainty data is not completely available for all isotopes and all reactions, [42]. Along with the gaps in uncertainties, the sensitivities are not as complete as well. Verification of which isotopes and how accurate the sensitivity and uncertainty data is for the available isotopes needs to be

conducted to ensure the software that uses this data will be valid.

The focus of this dissertation is to determine the sensitivity of the cross-sections on the K_{eff} , by perturbing the ENDF raw data in incremental steps. The new cross-sections will then be used in the calculations of the HMF-001 and HMF-004 experiments. This will be described in detail in the next chapter.

CHAPTER 3: METHODOLOGY

In order to accurately conduct and compute the research data, several requirements must be met to ensure all the software will integrate correctly and execute properly. This is to ensure that a cohesive and compatible set of data files are rendered as the desired output. The methodology for the research is broken down into six key areas. They are as follows:

- 1-Establish the platform for the computations, and conduct benchmarks. Make directory structure for MCNP6, MCNPX, MCNP_DATA, ENDF files, and NJOY files.
- 2-Download the raw ENDF data files from Brookhaven National Laboratory (BNL) servers, and determine appropriate sections for perturbation.
- 3-Create the Fortran code to perturb the appropriate sections of the files in varying amounts, (from 0.0001-30%, in incremented steps), using G95 Fortran compiler. Perturb the ENDF files.
- 4-Recombine the raw ENDF data file with the perturbed data and then format them into ACE I (MCNP6\X) formats, by using DOS batch scripts with the NJOY 2012.50 software.
- 5-Calculate the K_{eff} for the two different IHECSBE experiments, using MCNP6\X, with the baseline and perturbed cross-sections.
- 6-Using Excel, calculate the delta on K_{eff} for the two different IHECSBE experiments, (HMF-001 and HMF-004), analyzing K_{eff} versus percent perturbed.

These six steps will be the core of the research conducted. This chapter will address the step by step process to achieve these objectives.

1. A Microsoft Surface Pro 3 (SurfPro3) was selected as the machine of choice. It was chosen due to its compact size and multicore capabilities. It has 8 GB memory, an Intel i7-1.7 GHz core, 12-inch screen, and 512 MB SSD hard drive. It comes standard with Win10-x64bit version loaded. A Windows 10 platform was selected over Linux or Unix due to compatibility with all the required software. The required software also needed to run on the same machine, vice several different computers. This was a factor to prevent format errors in the files and any other inherent errors that could occur. All updates were conducted in Jan 2016 for the computer, and then the SurfPro3 was placed in airplane mode, to freeze the software updates.

The first software loaded was the G95 Fortran compiler file called G95-Mingw_201210.exe. This is a freeware GPU licensed Fortran compiler for Windows. This is required to be able to compile NJOY2012 and the self-made Fortran 95 perturbing program. G95 was selected over Intel Fortran Compiler (IFC), because Microsoft Visual Studio and numerous other C++ programs would have been required to be loaded as well. If these programs for IFC are not loaded in the correct order and manner, the compiler does not operate. Simplicity was chosen and G95 was the best option.

In order to enable multi-core processing capabilities, Microsoft's free software called HPC Pack 2012 MS-MPI program needed to be downloaded and executed. The file name is mpi_x64.msi. It installs a small program that tasks the cores separately and hyper-threads a single core, into two cores. This allows the running software to address a quad-core computer with 8-9 as many threads, depends on CLI settings. This greatly reduces the time required to complete calculations. The MS-MPI was installed, but once the clock times were analyzed for the MCNP6X runs, it was decided not to use the MPI versions of MCNP6 or MCNPX since the runs were so short, about an hour for 24 files.

After applying for a copy of the software from LANL T-2, the NJOY2012 zipfile was downloaded, with the appropriate license, see Appendix B. The software was unzipped and Update number 50 was applied, using the NJOY-provided UPD program. The final program was compiled using the standard commands for the G95 program, options are in the NJOY2012 eManual. A copy of the compiled program was set aside in case the primary program file became corrupted. All twenty test problems were executed with no issues, other than those already noted on the <http://t2.lanl.gov/nis/codes/NJOY12/> website.

After applying to RSICC for an individual license, the MCNP6\X software was received via DVD. The appropriate license is attached in Appendix C. The three-disc installation was simple and added all executables and data libraries in the correct locations on the Surface Pro 3's hard drive. Both MCNP6 and MCNPX 2.7.0 were installed under the C:\, as well as the MCNP_DATA. MCNP6 was installed in the C:\MCNP6 directory, while MCNPX was installed in the C:\MCNPX\ directory. All the Type I ACE formatted cross-sections and the XSDIR file is installed at C:\MCNP_DATA\. This provides the ability to run the benchmark models on both programs for comparison.

The XSDIR file is a text file that will require modification every time a new cross-section is added to the C:\MCNP_DATA\ directory. The XSDIR file is the index of all the available cross-sections in the MCNP_DATA directory. As new cross-sections are calculated, the XSDIR file is required to be updated or MCNP6\X will not know they are present or where they are located.

Test problems were executed on MCNP6 and MCNPX. No issues or deviations from previously recorded results were noted.

It is important to create a directory structure that will encapsulate all the created data.

Twelve sets of cross-sections will be required to show comparison in order test the perturbations. The *.50 and the *.86 series cross-sections were created with the ENDF/5 and ENDF/7B file formats respectively, and they come standard with the MCNP_DATA files. The *.70 cross-sections used the ENDF/7B data with the settings and NJOY2012.50 processing that all the other cross-sections will use. The *.70 set will be the baseline for comparison against the *.86 set. This will show deviations between the NJOY settings for BNL's ENDF cross-sections, and this research's settings. The *.71 through *.79 cross-sections are the perturbed sets of cross-sections.

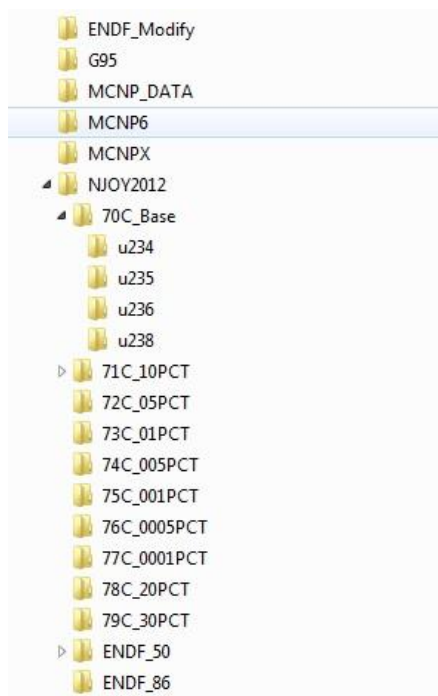
Table 7: Label Extensions for the Twelve Sets of Cross-Sections

Extension	Directory Name	Comment
*.50c	ENDF_50	This is the ENDF/B-5 format used originally calculating the CBE
*.86c	ENDF_86	This is the current ENDF/B-VI.8 that comes with MCNP6
*.70c	70C_Base	This is using the raw ENDF/B-VII.1 and NJOY2012.50 to make a Baseline
*.77c	77C_0001PCT	This is the +1.0001 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.76c	76C_0005PCT	This is the +1.0005 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.75c	75C_001PCT	This is the +1.001 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.74c	74C_005PCT	This is the +1.005 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.73c	73C_01PCT	This is the +1.01 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.72c	72C_05PCT	This is the +1.05 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.71c	71C_10PCT	This is the +1.1 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.78c	78C_20PCT	This is the +1.2 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50
*.79c	79C_30PCT	This is the +1.3 calculated perturbing using ENDF/B-VII.1 & NJOY2012.50

Each of the twelve directories, listed in Table 7, will require four subdirectories. These four subdirectories will be for each of the isotopes of concern, (U234, U235, U236, and U238). This is required in order to have a location to place the unperturbed ENDF file, the NJOY2012 DOS batch file, the NJOY2012 DAT file, and then the created NJOY2012 perturbed cross-section file. The NJOY program will also write a cross-section plot image, an output file, an XSDIR file, and Type I ACE cross-section file to this location as well. Figure 3 shows the basic

directory structure.

Figure 3: Directory Structure



A directory will also be required for the created Fortran code, that will perturb the unprocessed ENDF cross-sections. Create a directory in NJOY2012 labeled ENDF_MODIFY. The unprocessed ENDF files will be placed into this directory after downloaded from BNL's website, as well as the perturbed files will be written to this directory.

2. The four unprocessed ENDF files will be required to be downloaded from the NNDC's website, at <http://www.nndc.bnl.gov/exfor/endlf00.jsp>. An easy web interface is used to specify what isotope and which libraries (NLIB) to access. The main library of data that will be accessed will be the ENDF/B-VII.1 USA 2011 version (called NLIB1). This is the most current and complete of the US cross-section libraries, available from DOE's Brookhaven National

Laboratory. Do not download any other library or NJOY2012 may crash when executing. This is because multiple libraries will block the search feature in NJOY2012, and prevent it from finding the appropriate MF/MT sections for the desired MAT.

The four isotopes of concern are U-234, U-235, U-236, and U-238. These are the main materials of concern that are contained in the HMF-001 and HMF-004 evaluated experiments from the IHECSBE. No other isotopes need to be addressed for cross-section processing.

The ENDF file formats are available for many different incident particle types, called NSUBs. This is to provide the ability to select the exact type of particle reaction from many other different particle reactions. Understanding the scope of the research and the file formatting will assist you in limiting the amount of data that will be required for processing. As delineated previously in Chapter 2, the primary NSUBs for neutron interactions will be NSUB10 (Incident-Neutron Data). Many of the NSUBs do not have the capture, scattering, or absorption cross-section data associated with them. NJOY2012 needs those reactions and cross-sections in order to process the input files correctly.

NSUB10 satisfies the boundary condition of only iterating cross-sections for fission reactions. The other reactions will have no influence on establishing the sensitivities for the cross-sections, therefore they are not included in the processing. The modules in NJOY2012 require specific MFs and MTs from the raw ENDF file, and if not present when NJOY is executed, then the program will crash. Table 5 delineates the exact MF/MTs required for the appropriate NJOY module to work correctly. It is important to note that NSUB 4 and NSUB11 do not have the appropriate subsections to generate cross-section plots. NSUB0 has an energy range of 5 MeV to 20 MeV because it covers the photonuclear ranges, while NSUB10 is 1.0×10^{-10} MeV to 20 MeV.

Each of the isotopes of concern are associated with a designated Material number (MAT): U-234 is 9225, U-235 is 9228, U-236 is 9231, and U-238 is 9237. Accessing the BNL website and inputting the each of the isotopes/MATs into the input boxes will provide a selection of NSUBs, with MF and MT breakdowns, for each of the isotopes. There is the option-box to select all, some or only one of the NLIBs. The ENDF/B-VII.1 (NLIB1) was selected as it is the most current and complete of the NLIBs. It is also the easiest to use with the NJOY program.

By selecting the appropriate set of cross-sections, the webpage access will then allow the user to download the entire set of ENDF data points into a formulated text file. Figures 4 through 7 are examples of the webpage selection process for the three isotopes of interest.

Figure 4: NNBL ENDF Webpage for U-234

Request #26717

ENDF Data Selection

Retrieve Plot ☒ Selected ☐ Unselected ☐ All Reset

Plotting options: ☒ Quick plot (cross-sections only: σ)
☐ Universal plot ($\sigma \pm \Delta\sigma$, $d\sigma/d\Omega$, $d\sigma/dE$, $d^2\sigma/dE/d\Omega$) *beta version*

Sorted by: [Libraries] Reorder by: [Reactions] View: ☐ basic ☒ extended: get MAT, PEN, GND, run I

1)	Info	Summary	MAT	GND	PEN	Inter	92-U-234	MAT=9225	NSUB=0 (G)	20MeV	ENDF/B-VII.1
2)	Info	Summary	MAT	GND	PEN	Inter	92-U-234	MAT=3514	NSUB=4 (DECAY)		ENDF/B-VII.1
3)	Info	Summary	MAT	GND	PEN	Inter	92-U-234	MAT=9225	NSUB=10 (N)	30MeV	ENDF/B-VII.1
4)	Info	Summary	MAT	GND	PEN	Inter	92-U-234	MAT=9225	NSUB=11 (N/FPY)	20MeV	ENDF/B-VII.1

Figure 5: NNBL ENDF Webpage for U-235

Request #26719

ENDF Data Selection

Retrieve Plot ☒ Selected ☐ Unselected ☐ All Reset

Plotting options: ☒ Quick plot (cross-sections only: σ)
☐ Universal plot ($\sigma \pm \Delta\sigma$, $d\sigma/d\Omega$, $d\sigma/dE$, $d^2\sigma/dE/d\Omega$) *beta version*

Sorted by: [Libraries] Reorder by: [Reactions] View: ☐ basic ☒ extended: get MAT, PEN, GND, run I

1)	Info	Summary	MAT	GND	PEN	Inter	92-U-235	MAT=9228	NSUB=0 (G)	20MeV	ENDF/B-VII.1
2)	Info	Summary	MAT	GND	PEN	Inter	92-U-235	MAT=3515	NSUB=4 (DECAY)		ENDF/B-VII.1
3)	Info	Summary	MAT	GND	PEN	Inter	92-U-235	MAT=9228	NSUB=10 (N)	20MeV	ENDF/B-VII.1
4)	Info	Summary	MAT	GND	PEN	Inter	92-U-235	MAT=9228	NSUB=11 (N/FPY)	20MeV	ENDF/B-VII.1
5)	Info	Summary	MAT	GND	PEN	Inter	92-U-235	MAT=9228	NSUB=19 (Std)	200MeV	ENDF/B-VII.1

Figure 6: NNBL ENDF Webpage for U-236

Request #26720

ENDF Data Selection

Retrieve Plot ☒ Selected ☐ Unselected ☐ All Reset

Plotting options: ☒ Quick plot (cross-sections only: σ)
☐ Universal plot ($\sigma \pm \Delta\sigma$, $d\sigma/d\Omega$, $d\sigma/dE$, $d^2\sigma/dE/d\Omega$) *beta version*

Sorted by: [Libraries] Reorder by: [Reactions] View: ☐ basic ☒ extended: get MAT, PEN, GND, run I

1)	Info	Summary	MAT	GND	PEN	Inter	92-U-236	MAT=9231	NSUB=0 (G)	20MeV	ENDF/B-VII.1
2)	Info	Summary	MAT	GND	PEN	Inter	92-U-236	MAT=3517	NSUB=4 (DECAY)		ENDF/B-VII.1
3)	Info	Summary	MAT	GND	PEN	Inter	92-U-236	MAT=9231	NSUB=10 (N)	30MeV	ENDF/B-VII.1
4)	Info	Summary	MAT	GND	PEN	Inter	92-U-236	MAT=9231	NSUB=11 (N/FPY)	20MeV	ENDF/B-VII.1

Figure 7: NNBL ENDF Webpage for U-238

Request #26721

ENDF Data Selection

Retrieve Plot ☒ Selected ☐ Unselected ☐ All Reset

Plotting options: ☒ Quick plot (cross-sections only: σ)
☐ Universal plot ($\sigma \pm \Delta\sigma$, $d\sigma/d\Omega$, $d\sigma/dE$, $d^2\sigma/dE/d\Omega$) *beta version*

Sorted by: [Libraries] Reorder by: [Reactions] View: ☐ basic ☒ extended: get MAT, PEN, GND, run I

1)	Info	Summary	MAT	GND	PEN	Inter	92-U-238	MAT=9237	NSUB=0 (G)	20MeV	ENDF/B-VII.1
2)	Info	Summary	MAT	GND	PEN	Inter	92-U-238	MAT=3519	NSUB=4 (DECAY)		ENDF/B-VII.1
3)	Info	Summary	MAT	GND	PEN	Inter	92-U-238	MAT=9237	NSUB=5 (S/FPY)		ENDF/B-VII.1
4)	Info	Summary	MAT	GND	PEN	Inter	92-U-238	MAT=9237	NSUB=10 (N)	30MeV	ENDF/B-VII.1
5)	Info	Summary	MAT	GND	PEN	Inter	92-U-238	MAT=9237	NSUB=11 (N/FPY)	20MeV	ENDF/B-VII.1
6)	Info	Summary	MAT	GND	PEN	Inter	92-U-238	MAT=9237	NSUB=19 (Std)	200MeV	ENDF/B-VII.1

By selecting only NSUB10, a text file of the associated data, including all the cross-sections, will be available for retrieval or download. Select and download the file, saving it with a distinct nomenclature. The naming structure for the raw data file was u234_nlib1_nsub10.txt. This clearly designated what was contained in the file. Place the four data files in the ENDF_Modify directory.

The MT sections that are required to be processed are as follows: MT1-Total Cross section, MT2-Elastic Cross section, MT3-Nonelastic Cross section, MT4-Inelastic Cross section, MT18-total fission cross-section, MT19-first chance fission (n,f), MT20-second chance fission (n,n'f), MT21-third chance fission (n,2nf), and MT38-fourth chance fission (n,3nf). The Total cross-section MT1 is a sum of MT2 and MT3. The data in MT18 is the sum of the data in MT19, MT20, MT21, and MT38.

The downloaded files can range in size from a few kilobytes to tens of megabytes. The download process will be required for each of the isotopes of interest, U-234, U-235, U-236, and U-238. The four downloaded raw ENDF text files are readable in Notepad or Wordpad, but Wordpad is recommended for the larger files above 1 MB. Use the Landscape Orientation when viewing or modifying the files. Any work done on these files must keep the file in the original ASCII TXT format, or NJOY2012 will not be able to process it.

In order to improve the efficiency of the Fortran perturbing code, it is essential to identify the sections of the raw ENDF file that requires processing. The Fortran program to perturb the cross-sections will remove columns 67-80 and not replace them. These are the MAT/MF/MT and row numbers that are required for NJOY2012 to find the appropriate sections of the ENDF file to process. This will require hand-typing the data fields back into each of the rows. This is required

to replace the perturbed cross-sections back into the locations where they were cut and copied.

Table 8: ENDF File Contents

U234_MOD.TXT	NSUB	MF	MT	E- σ PAIRS	Row start	Row stop
	10	3	1	439	4	151
			2	439	155	302
			3	439	306	453
			4	255	457	542
U234_MOD2.TXT			18	355	4	123
			19	355	127	246
			20	282	250	344
			21	145	348	397
			38	87	413	442
U235_MOD.TXT	10	3	1	361	4	125
			2	361	129	250
			3	361	254	375
			4	307	379	482
U235_MOD2.TXT			18	313	4	109
			19	313	113	218
			20	61	222	243
			21	37	247	260
			38	18	270	276
U236_MOD.TXT	10	3	1	307	4	107
			2	307	111	214
			3	306	218	320
			4	233	324	402
U236_MOD2.TXT			18	242	4	85
			19	242	89	170
			20	149	174	224
			21	69	228	251
			38	41	269	283
U238_MOD.TXT	10	3	1	395	4	136
			2	395	140	272
			3	395	276	408
			4	175	412	471
U238_MOD2.TXT			18	287	4	100
			19	287	104	200
			20	87	204	233
			21	64	237	259
			38	49	277	294

It was determined that MF3 and sections MT1-4, 18-21, and 38 were the sections requiring perturbation. These MT sections can be cut and copied out of the main raw ENDF file in two parts and saved as u23N_mod.txt (for MT1-4) and u23N_mod2.txt, (for MT18-21, 38). The N is replaced with 4,5,6, or 8 in the filename for each of the different isotopes. The same process is done for the other three isotopes.

Table 8 lists the pertinent sections of the contents of the required files for modification, and the row numbers for ease of programming. This also gives an indication of how many rows will require MAT/MF/MT and row number replacements. Table 8 is also a good source for conducting a “checksum” verification of how many rows will be renumbered.

Along with the raw ENDF files, the plots of the baseline energy to cross-sections are also available on the same webpage. Figures 8 through 11 display the baseline cross-section for all four isotopes. The visualization of the plots clearly indicate that each isotope is unique.

Figure 8: ENDF Baseline Energy-Vs-Cross-sections graph for U-234

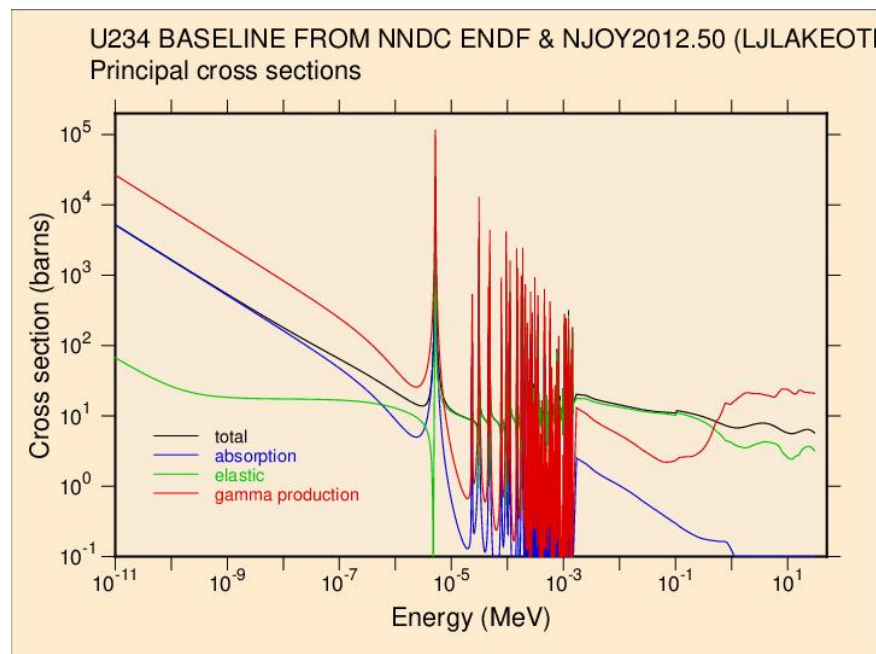


Figure 9: ENDF Baseline Energy-Vs-Cross-sections graph for U-235

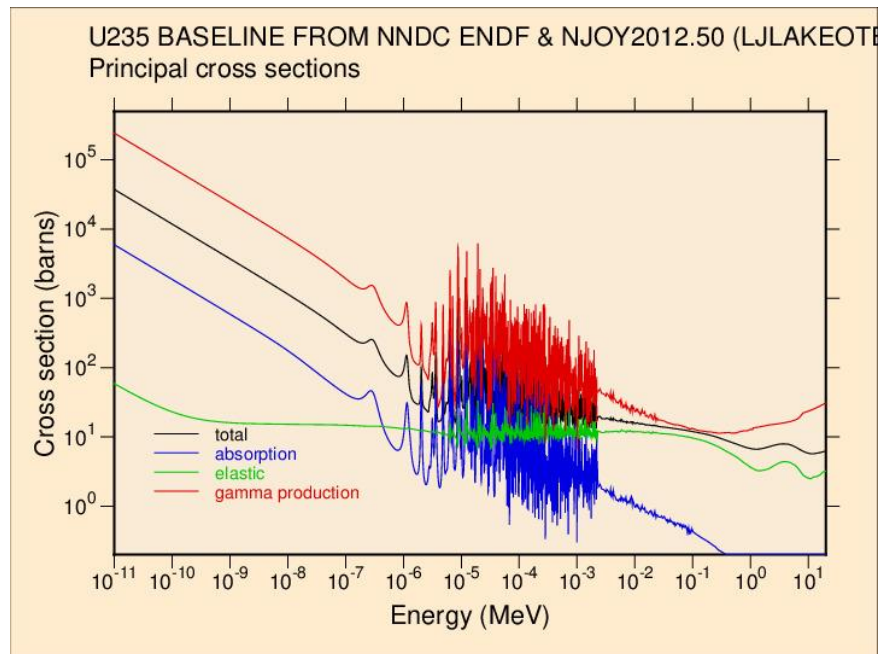


Figure 10: ENDF Baseline Energy-Vs-Cross-sections graph for U-236

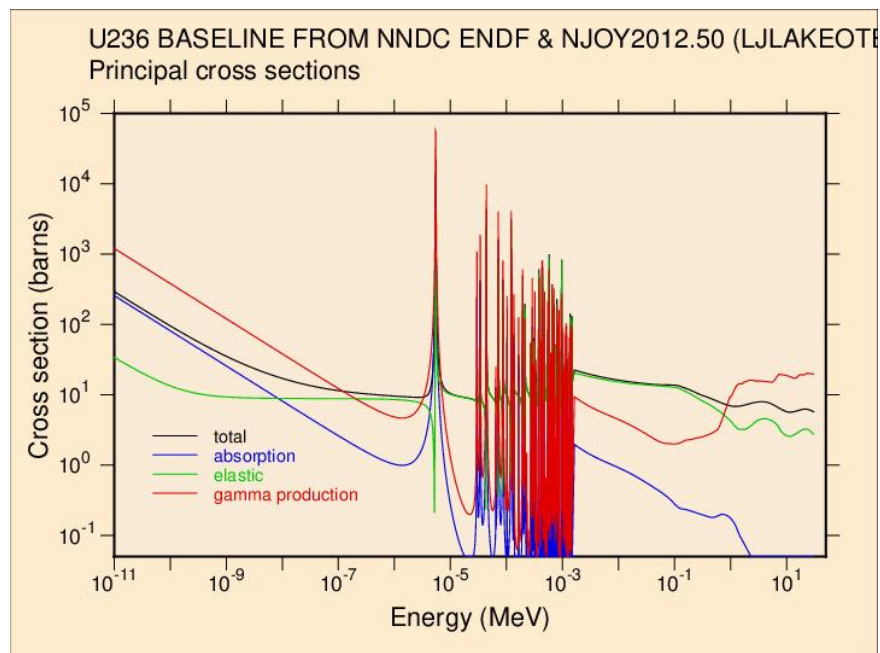
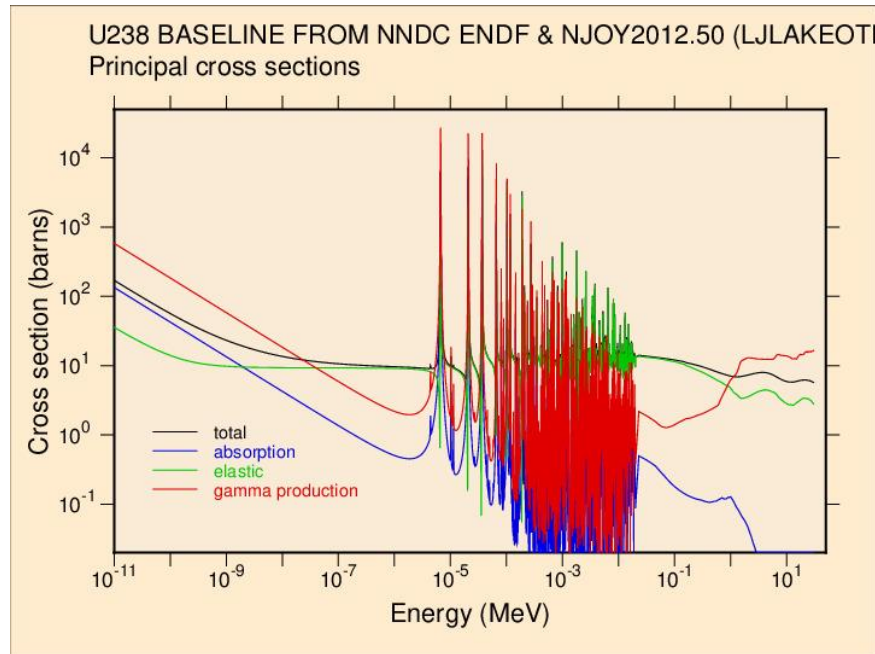


Figure 11: ENDF Baseline Energy-Vs-Cross-sections graph for U-238



3. Creating the FORTRAN 95 code for the perturbation of the raw ENDF data required the installation of the G95 FORTRAN compiler. This was accomplished in Step 1. This should not be a complicated program. It can easily run as a CLI program, with no GUI interface. This will keep the code simple and small.

An understanding of the exact construction of the ENDF file is required in order to correctly parse out sections of the raw ENDF file and properly replace them with modified sections from the Fortran perturbation code. Since we are only dealing with MF3, (sections MT 1-4 and MT18-38), this greatly simplifies the process. Each MF section is structured differently, so staying within the same MF will allow a common template for perturbing and replacement of only the cross-sections.

Table 9: ENDF Material File 3/MT Structure

Columns									
1-11	12-22	23-33	34-44	45-55	56-66	67-70	71-72	73-75	76-80
MAT #	AWR	0	0	0	0	MAT	MF	MT	ROW #1
0.0	0.0	0	0	LR=1	E/ σ PAIRS	MAT	MF	MT	ROW #2
E/ σ PAIRS	PAIR=2					MAT	MF	MT	ROW #3
ENERGY	σ	ENERGY	σ	ENERGY	σ	MAT	MF	MT	ROW #4
~	~	~	~	~	~	~	~	~	~
ENERGY	σ	ENERGY	σ	ENERGY	σ	MAT	MF	MT	ROW# N-1
ENERGY	σ	ENERGY	σ	ENERGY	σ	MAT	MF	MT	ROW# N
0.0	0.0	0	0	0	0	MAT	MF	MT	99999

The structure for MF3/MT1-4 and MT18-38 is as delineated in Table 9. Each of the first three rows and the last row are the headers and footers to the MT section. These are required so the NJOY2012 software can correctly find and use the appropriate data. They cannot be modified. Each MT is different from the others, because the MF sections hold different data on the nuclear structure and reactions, so the Fortran code must be made specifically for the MF3 section of the ENDF file.

The reader will need to know and understand where all the headers and footers for each section are, so that they can be repaired/corrected/QC'd after the MT section is perturbed. This is done by ensuring that they match the headers and footers of the MT sections before they were perturbed, as well as ensuring that all MAT/MF/MT and rows are added back on in columns 67-

80.

Use Excel to import the text file into a spreadsheet. This will give you an accurate count of how many rows you there are per section. This is how the Table 8 data was obtained for all the MT sections.

Now that the row structure is understood, it is important to comprehend the column structure. Table 9 also displays the columns for the MT sections. There will be three energy-cross-section pairs per row. Each pair is 11x11 columns, with the first 11 being the energy, (not to be perturbed) and the second 11 being the cross-section, (to be perturbed). This translates into the display of Table 10, with sections being constant and others perturbed or erased.

Originally the code was designed for four tasks. They are to make a “Master Table” of the isotopes, generate new perturbed ENDF cross-section files from the “Master Table”, generate a single perturbed ENDF cross-section file, or generate a “Demo” file for practicing making cross-sections. Each of these tasks has its’ own section of code, and several that overlap. The main task of generating a single ENDF perturbed file is the priority for the research, so this will be the area of detailed descriptions.

Simplicity is the key, so writing the program for only what is needed is an important boundary condition. The requirements for creating the Fortran code are as follows:

- enable a file read/select so the code can fetch the correct data (F_IN),
- enable a row selection so the code knows where to start (L_STR),
- enable a row stop, so the wrong data doesn’t get perturbed (L_END),
- request how much to perturb the cross-sections (XLM),
- enable a write feature so the code is directed to where to save the data (F_OUT).

It is a simple matter to write the code to ask for a file name as input, and then store it as a

variable (F_IN). To keep the Fortran perturbation program as simple as possible, the input file needs to be in the same directory as the program, otherwise more code will be required to instruct the program to change directories to look for the file. It is just as simple to ask and write the output file name (F_OUT).

Table 10: Perturbed ENDF File

Columns						
1-11	12-22	23-33	34-44	45-55	56-66	67-80
ENERGY (keep)	σ (perturb)	ENERGY (keep)	σ (perturb)	ENERGY (keep)	σ (perturb)	MAT/MF/MT/Row (Erased)
XCOM1	XCOM2	XCOM3	XCOM4	XCOM5	XCOM6	

The program is directed to look at the file, (located by name by F_IN). The starting row (L_STR) will be loaded into memory (A). The row will be divided up the sections (XCOM1) through (XCOM6). Each variable (XCOM) will be F11.4 in size. Table 10 shows the location of the XCOM variables.

A linear multiplier (XLM) will be request as input from the user. This multiplier will be stored in memory and used with select XCOM variables. It is a F6.4 variable integer (N.NNNN) inputted by the user in the initial screen questions. Variables XCOM2, XCOM4, and XCOM6 will have the multiplier (XLM) used prior to being written into the new file (F_OUT). Variables XCOM1, XCOM3, and XCOM5 will pass through with no multiplier applied. All six XCOM variables will then be placed back in numerical order and written in the new file (F_OUT). The program will retrieve the next row (ICOUNT+1), until the row count equals the max rows requested for perturbing (L_END). After the program has written the last row to the new file, it terminates.

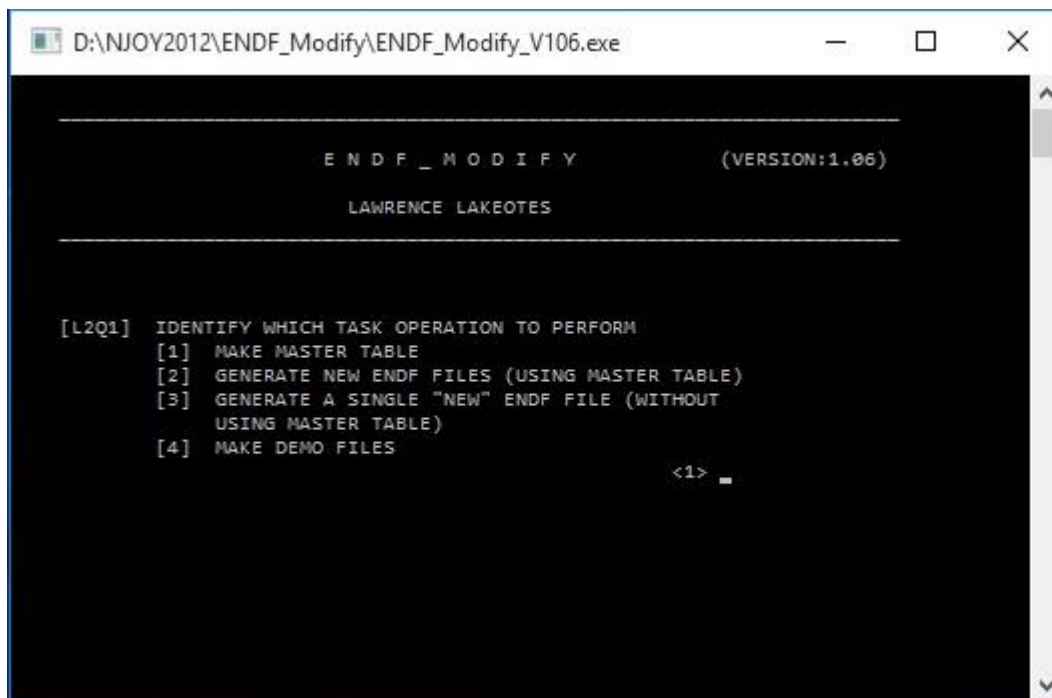
Since the six sections of 11 columns will only equal 66, everything from column 67 to 80 will be dumped. This is the MAT/MF/MT and row numbers. This is why they must be manually entered after the MT section is perturbed.

This is the basics of the Fortran perturbation program. It is a bit more complicated than what is written here, but has been simplified. It took several tries and a few changes in features in order to get the ENDF Modify code to successfully execute the desired commands. Fortran is not a commonly used language, but it was the simplest to program and compile. The full complete copy of the program is in Appendix D.

By using the five simple steps listed above, a 21kb file was created. It was written in NotePad, and then saved as ENDF_ModifyV106.for. G95 Fortran compiler was used with the standard settings and the output was ENDF_ModifyV106.exe. The output file was 373 kB, and executable in a DOS Box in Windows. The executable file was copied into the ENDF_Modify directory. This allows the program direct access to the ENDF files that require perturbing.

Now that the ENDF_ModifyV106.exe and the ENDF files are in the same directory, it is time to start perturbing the ENDF files. It is important to perturb the isotopes in order and by the same percent for all four isotopes before moving onto the next percent perturbation. This means perturbing U234, U235, U236, and U238 all for the 1.10 multiplier, before moving onto the next iteration of perturbation. Figure 12 shows the opening screen for the ENDF_ModifyV106.exe program. Figure 13 shows all the options filled out for making a single perturbed ENDF file for U234 at 1.10 multiplier, or +10% perturbing.

Figure 12: Opening screen of ENDF_ModifyV106.exe



```

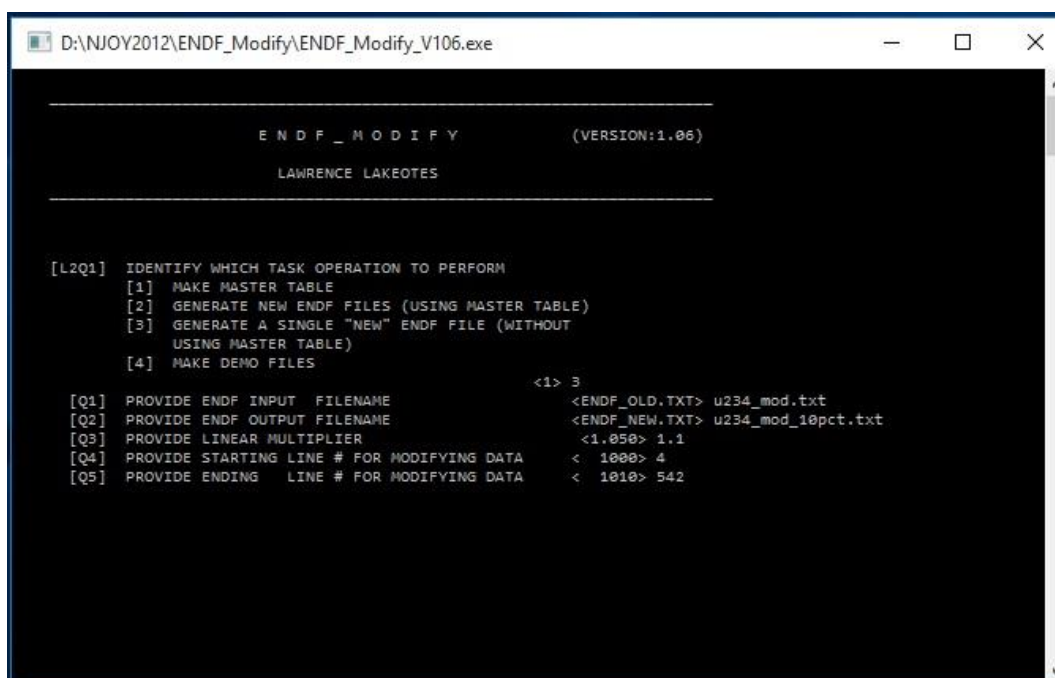
D:\NJOY2012\ENDF_Modify\ENDF_Modify_V106.exe

-----
E N D F _ M O D I F Y          (VERSION:1.06)
LAWRENCE LAKEOTES
-----

[L2Q1] IDENTIFY WHICH TASK OPERATION TO PERFORM
      [1] MAKE MASTER TABLE
      [2] GENERATE NEW ENDF FILES (USING MASTER TABLE)
      [3] GENERATE A SINGLE "NEW" ENDF FILE (WITHOUT
           USING MASTER TABLE)
      [4] MAKE DEMO FILES

           <1> _
```

Figure 13: Completed ENDF_ModifyV106.exe Screen



```

D:\NJOY2012\ENDF_Modify\ENDF_Modify_V106.exe

-----
E N D F _ M O D I F Y          (VERSION:1.06)
LAWRENCE LAKEOTES
-----

[L2Q1] IDENTIFY WHICH TASK OPERATION TO PERFORM
      [1] MAKE MASTER TABLE
      [2] GENERATE NEW ENDF FILES (USING MASTER TABLE)
      [3] GENERATE A SINGLE "NEW" ENDF FILE (WITHOUT
           USING MASTER TABLE)
      [4] MAKE DEMO FILES

           <1> 3

[Q1] PROVIDE ENDF INPUT FILENAME          <ENDF_OLD.TXT> u234_mod.txt
[Q2] PROVIDE ENDF OUTPUT FILENAME         <ENDF_NEW.TXT> u234_mod_10pct.txt
[Q3] PROVIDE LINEAR MULTIPLIER             <1.050> 1.1
[Q4] PROVIDE STARTING LINE # FOR MODIFYING DATA < 1000> 4
[Q5] PROVIDE ENDING LINE # FOR MODIFYING DATA  < 1010> 542
```

As soon as the four isotopes are individually perturbed for one iteration, it is a good time to copy all four of the newly modified ENDF files into the appropriate perturbed directory, (i.e. the 10% directory for a 1.1 multiplier). Conduct this process on all four isotopes for multipliers 1.0001, 1.0005, 1.001, 1.005, 1.01, 1.05, 1.1, 1.2, and 1.3 for each MT section that is required. Ensure that the set of four ENDF perturbed isotope files are copied to the appropriate perturbed directory.

When MT sections 1-4 and 18-38 are completely perturbed for all four isotopes, it is time to fill in all the MAT/MF/MT and row numbers for all the perturbed files. This will take some time, but NJOY2012 will not work otherwise. It takes about an hour to hand type in the numbers for a single iteration of perturbation, (containing four isotopes).

4. After the MT sections have had all the MAT/MF/MT and row numbers added back in, then it is time to cut and copy them back into the original files downloaded from NNDC. Ensure there is an original file ENDF file and the corrected/perturbed MT files in each isotope subdirectory of each iteration directory. Replace the MT sections in the NNDC downloaded file with the new and perturbed MT sections MT1-4 and MT18-38.

The new modified ENDF file shall be named u23N_nlib1_nsub10_mod.txt, where the word “mod” is replaced with the perturbation amount, and the u23N is the appropriate isotope for this perturbation. This is the input data file for NJOY2012 to be able to create a set of Type I ACE file cross-sections.

This is done for all nine sets of perturbed cross-sections, containing four isotopes each. A total of 36 modified ENDF files will require QC review to ensure that all the numbers are

correctly filled in and that the cross-sections are actually perturbed by the desired amount. Hand calculations were conducted on every isotope for every iteration to validate this requirement.

At this point, there should be a correctly modified ENDF file in every isotope subdirectory in the NJOY2012 main directory, each one placed under one of the ten appropriate iteration directories. Verify all subdirectories in NJOY have a ENDF file before proceeding to the next step.

The NJOY2012.50 program is already installed and updated. It is time to create the a NJOY2012 DOS Batch file to execute the individual DAT files for each of the 40 different sets of cross-sections that will have to be processed. It is very important that all 40 batch and DAT files be identical, except for the file extension, isotope and incremental perturbed amount. This will provide uniformity in processing all the cross-sections as well as simplicity. A full copy of the DOS batch file for U234 for the baseline cross-sections (*.70) is in Appendix E.

The DOS batch file first copies and renames the modified ENDF file into a filename called "tape20." This tape is placed into the same perturbed_amount/isotope directory as the DOS batch file, DAT file, and modified ENDF file. The next command in the batch file is the execute command for NJOY2012 program. The input file for the NJOY executable is the DAT file for that perturbed amount and isotope.

The next command in the batch file will be executed after the NJOY program has terminated. The next five commands will rename five output/tape files. The five files are the output, XSDIR, plot, PENDF, and cross-section file. The contents of the XSDIR file will go into the contents of the master XSDIR file in the MCNP-DATA directory.

The newly created cross-section file will be copied in the next step into the MCNP-DATA directory, to become part of the library for the MCNP6\X programs. The cross-section file is

named by the atomic number (Z) plus the mass number (A) plus the extension (*.7Nc), so that the final product is “ZA.7Nc”. The extension is dependent upon the series of iterations that the cross-section was processed under. Review Table 7 for a cross-references of extensions to perturbed amounts.

The last three commands in the batch file deletes the excess tapes created by the NJOY program. These tapes are necessary for the processing of the modified cross-section, but have no bearing on the process when the NJOY program terminates. Deleting these files saves on hard drive space.

Now that the basic template is created, change the extension, isotope, and percent perturbed for each of the other 39 DOS batch files required to be created. Place each of the DOS batch files in the appropriate subdirectory following the perturbed amount and then isotope directory structure.

The next step in getting NJOY2012 to run is to create the DAT file. The DAT file is the list of modules, with parameters, that NJOY2012 will run in order to process the modified ENDF file into a useful set of cross-sections. Appendix F contains examples of DAT files for all four isotopes for the baseline. The modules need to be ran in order or the cross-sections will not get constructed correctly, and NJOY2012 will crash. The modules are all set with defaults and for 300K in temperature.

The MODER module is the first one in the DAT file. It converts the ASCII text file into binary, to speed up the processing speed. The RECONR module is the next module that will reconstruct resonance cross-sections from resonance parameters and nonlinear interpolation schemes. The third module is BROADR, and it generates Doppler-broadened cross-sections.

The next module is UNRESR module, and it produces effective self-shielded cross-

sections for the resonance reactions, in the unresolved energy range, from the output of the previous module. The ENDF file has the resonances averaged in the resonance range, and NJOY2012 will convert that into effective cross-sections by the Bondarenko method, [27]. This method requires the use of an “effective escape” cross-section, which is the probability that a neutron may escape a resonance by leaving a region.

The next module is HEATR and it generates radiation damage energy production and point-wise heat production cross-sections for specific reactions. The sixth module is THERMR and its purpose is to generate pointwise neutron scattering cross-sections in the thermal energy range. GASPR is the next module and adds gas-productions (MT203-MT207) to the PENDF file. The PURR module creates a table for the unresolved resonance self-shielded data, because Monte Carlo codes have difficulty interpreting the cross-sections in this energy range.

MODER will convert the PENDF data back from binary to ASCII text, so that the ACER module can properly create the output file, the cross-section, the XSDIR and cross-section Plot. All the created files will be in the same directory as the DAT and batch file.

Once the first DAT file is complete, it will be easy to change the extension, MAT number, and percent perturbed for each of the other 39 DAT files required to be created. Place each of the DAT files in the appropriate subdirectory.

All the preparatory steps are complete in order to execute the NJOY2012 program. Ensure the update has been applied. This can be found at <http://t2.lanl.gov/nis/codes/NJOY12/>. A master batch file could easily be created to run all the subordinate batch files, but it is better to observe the individual batch files running to ensure no crashes occur. APPENDIX G has the example of the Master NJOY DOS batch file, if that path is desired.

Start with the baseline cross-section and run the DOS batch files for all 40 DOS batch

files, one at a time. Verify that all the DOS batch files executed correctly and all subdirectories in NJOY2012 have the correctly named output, PENDF, cross-section, XSDIR and plot files. If they do not, it is a symptom of a crashed NJOY2012 program due to a bad DAT or batch file.

5. After the NJOY2012 program has created the new Type I ACE files and XSDIR entries for each of the 40 different cross-sections, it is time to combine those in the current MCNP_DATA directory and make a new XSDIR index file from the current one.

In each of the 40 different NJOY2012 subdirectories, there are two important files that must be copied and relocated. They are the new individual XSDIR file and the numbered continuous energy cross-section file (the “ZA.7Nc” file).

The Master XSDIR file is in the MCNP_DATA directory. The first half of the file contains a list of all the AWRs for all isotopes, and the second half of it contains an index of all the cross-sections contained in the MCNP_DATA directory. Any cross-section referenced or needed by the MCNP6/X program must reside in the same directory as the XSDIR file.

Make a copy of the Master XSDIR file in any other location but MCNP_DATA. This will ensure that the MCNP_DATA directory can be restored to original structure after this research. Move all files in the MCNP_DATA directory that contain the name “XSDIR” in it to a temporary directory, so that the MCNP6/X program must reference only the Master XSDIR file that is being modified.

Open the Master MCNP_DATA\XSDIR file in a text file reader (i.e. NotePad). Remove all but the following rows in the second half of the XSDIR line: 92234.50c, 92235.50c, 92236.50c, 92238.50c, 92234.86c, 92235.86c, 92236.86c, 92238.86c, 1001.50c, 6000.50c, 7014.50c, 8016.50c, 13027.50c, and lwtr.01t. Save the file, but keep it open, so the new XSDIR

rows can be added from the created NJOY2012 XSDIR files.

Just like executing the NJOY2012 program, it is easiest to go through each of the isotopes in a perturbed iteration before moving on to the next iteration. Start with the baseline iteration (*.70c) and the U-234 isotope, and copy the cross-section file from the 70C_Base\u234 subdirectory into MCNP_DATA directory, where the Master XSDIR file is located. Open the u234_basexsdir.txt file in a text file reader (i.e. NotePad) and copy the one line of text, and then close the file. Open the Master XSDIR file and paste the line of text under the second half of the file, after the word “directory.”

Do these two steps for all 40 processed cross-sections. When complete, there should be 40 new cross-sections (*.70 through *.79) in the MCNP_DATA directory. There should now be only 54 lines of text in the second half of the XSDIR file. Edit the 40 additional lines in the second half of the Master XSDIR file, by replacing the word “filename” with the ZA.7N.c designation that is at the beginning of each of the line. This is the filename of the cross-section file associated with that line in the XSDIR file. Also, replace the word “route” in each line with the number 0. This is required by MCNP6/X in order to use and access the cross-section as a Type I ACE formatted cross-section file. Appendix I shows an example of a correctly edited second half of the Master XSDIR file. Save and close the Master XSDIR file. All modifications and corrections to the MCNP_DATA directory are complete.

The first step to completing the MCNP6\X portion of the research is to copy the HMF-001 and HMF-004 text files from the IHECSBE and make two new text files in the MCNP6\Bin directory. These will be named the HMF_001_50.txt and HMF_004_50.txt files. They are the experimental comparisons, that will be used as the benchmark against all the perturbed iterations. Appendix J is the copy of the two MCNP decks.

Copy the two MCNP files and rename them as HMF_001_86.txt and HMF_004_86.txt. Edit the Material Cards in the third section of each deck, and replace the *50c extension with the *.86c extension on the 92234, 92235, 92236, and 92238 for both files. Save the files.

Copy both the HMF_001 and HMF_004 files again and repeat the above process for the *.70c, *.71c, *.72c, *.73c, *.74c, *.75c, *.76c, *.77c, *.78c, and *.79c extensions. After completion of this task, there should be a total of twelve HMF_001 and twelve HMF_004 text files within the MCNP6\bin directory. Copy all 24 MCNP files and place a copy of them into the MCNPX\bin directory. This will allow the comparison between the two Monte Carlo codes.

The last step required to complete the circuit is to establish the MCNP6\X master DOS Batch file. The master DOS batch file lists the individual files to execute. There will be the 24 files to be run in MCNP6 and then MCNPX. Appendix K shows the text from both of the Master MCNP6 and MCNPX batch files. The batch file is called phd.bat in both Monte Carlo codes. Execute both batch files, one at a time, and observe the outputs. Correct any issues and rerun the batch file, if required. There should be 24 output files in each of the MCNP6\bin and MCNPX\bin directories.

6. After MCNP6 and MCNPX has executed all 48 runs, it is time to extract the pertinent data. Make a copy of the 24 output files in each of the MCNP6\bin and MCNPX\bin directories and place them on the Desktop. This will greatly ease the access to the data and speed the processing of the results. This completes the Methodology of the process to perturb cross-sections.

CHAPTER 4: FINDINGS OF THE STUDY

Four ENDF formatted files were downloaded from the BNL website. These are the basic isotope ENDF files, from which all the modified and processed cross-sections are derived. Thirty-six cross-sections were modified from the four basic ENDF files, using the Fortran95 perturbation program. The 36 files were also hand-renumbered to ensure that the MT sections were replaced back into the correct location, in the original ENDF formatted files. This process now resulted in the creation of 36 modified ENDF formatted files. The modified files were placed into the appropriate perturbed and isotope directories in the NJOY2012 folder. The modified ENDF files were compared to the unmodified files and then validated with hand calculations. The comparisons were accomplished prior to executing the NJOY2012 program.

The difference between the 40 generated files and the 36 modified files was that a standard ENDF/B-VII.1 set of cross-sections (containing one file each of U-234, U-235, U-236, and U-238) were generated with no perturbing. This was the cross-section set with the extension of *.70c. This is the true baseline of all nine sets of the modified cross-sections. Extensions *.50c and *.86c were cross-sections from previously created NJOY cross-sections. Those sets are already contained in the MCNP_DATA folder from the installation program. The *.70c and *.86c should be within one sigma in difference when calculating the MCNP6 benchmarks, (and they are).

The NJOY2012 program successfully imported all 40 of the ENDF files and generated the Type I ACE formatted cross-sections for the unmodified and perturbed U-234, U-235, U-236, and U-238 isotopes. All of the iterations were correctly computed and placed in the appropriate MCNP_DATA directory, for reference by the Monte Carlo codes. The XSDIR file was updated

with the new rows containing the new cross-section data from the NJOY2012 XSDIR output files. The MCNP_DATA directory now contains all the files and modifications required to run the MCNP6\X codes.

Table 11: Comparison of Benchmarks from MCNP6

MCNP6 ENDF Series	Comments	Iteration	HMF- 001 MT1-4	HMF- 004 MT1-4	HMF- 001 MT1-38	HMF- 004 MT1- 38
			K_{eff}	K_{eff}	K_{eff}	K_{eff}
Actual	This is the experimental measurements in the lab.	0.0000	1.0000	0.9985	1.0000	0.9985
Calc	This is MCNP5 and ENDF/B-VI.8 from IHECSBE	0.0000	0.9966	0.9948	0.9966	0.9948
*.50c	This is the ENDF/5 format used originally calculating the CBE	0.0000	0.99745	0.99734	0.99745	0.99734
Calc	This is MCNP5 and ENDF/B-VII B3 from IHECSBE	0.0000	1.0000	1.0003	1.0000	1.0003
*.86c	This is the current ENDF/B-VII.1 that comes with MCNP6	0.0000	0.99988	1.00350	0.99988	1.00350
*.70c	This is the current ENDF/B-VII.1 using NJOY2012.50 (Baseline)	0.0000	1.00006	1.00416	1.00006	1.00416
*.77c	This is the +1.0001 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0001	0.99949	1.00343	1.00083	1.00286
*.76c	This is the +1.0005 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0005	0.99972	1.00352	1.00071	1.00341
*.75c	This is the +1.001 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0010	1.00027	1.00328	1.00145	1.00583
*.74c	This is the +1.005 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0050	1.00054	1.00540	1.00419	1.00678
*.73c	This is the +1.01 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0100	1.00073	1.00361	1.00767	1.00883
*.72c	This is the +1.05 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0500	1.00506	1.00632	1.03880	1.03192
*.71c	This is the +1.1 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.1000	1.01103	1.00843	1.07573	1.06180
*.78c	This is the +1.2 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.2000	1.02217	1.01450	1.14698	1.11373
*.79c	This is the +1.3 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.3000	1.03203	1.01901	1.21463	1.16652

A total of forty-eight files of MCNP6 and MCNPX decks were calculated to analyze the perturbing effect on the cross-sections for a well-known experimental benchmarks. The MCNP6

and MCNPX software executed as programmed using the new 40 cross-sections. Since both codes tracked together, as seen in Figure 14, MCNP6 will be primarily the referenced neutronic code.

Table 12: Comparisons of Benchmarks from MCNPX

MCNPX 2.7.0 ENDF Series	Comments	Iteration	HMF-001 MT1-4	HMF-004 MT1-4	HMF-001 MT1-38	HMF-004 MT1-38
			K_{eff}	K_{eff}	K_{eff}	K_{eff}
Actual	This is the experimental measurements in the lab.	0.0000	1.0000	0.9985	1.0000	0.9985
Calc	This is MCNP5 and ENDF/B-VI.8 from IHECSBE	0.0000	0.9966	0.9948	0.9966	0.9948
*.50c	This is the ENDF/5 format used originally calculating the CBE	0.0000	0.99761	0.99522	0.99761	0.99522
Calc	This is MCNP5 and ENDF/B-VII B3 from IHECSBE	0.0000	1.0000	1.0003	1.0000	1.0003
*.86c	This is the current ENDF/B-VII.0 that comes with MCNP6	0.0000	1.00055	1.00377	1.00055	1.00377
*.70c	This is the current ENDF/B-VII.1 using NJOY2012.50 (Baseline)	0.0000	1.00023	1.00277	1.00023	1.00277
*.77c	This is the +1.0001 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0001	0.99952	1.00286	0.99966	1.00259
*.76c	This is the +1.0005 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0005	1.00017	1.00272	1.00014	1.00385
*.75c	This is the +1.001 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0010	0.99958	1.00285	1.00103	1.00450
*.74c	This is the +1.005 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0050	1.00063	1.00422	1.00380	1.00727
*.73c	This is the +1.01 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0100	1.00138	1.00429	1.00743	1.00924
*.72c	This is the +1.05 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.0500	1.00592	1.00545	1.03809	1.03158
*.71c	This is the +1.1 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.1000	1.01104	1.00790	1.07609	1.05994
*.78c	This is the +1.2 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.2000	1.02220	1.01223	1.14633	1.11485
*.79c	This is the +1.3 calculated perturbation using ENDF/B-VII.1 & NJOY2012.50	1.3000	1.03294	1.01785	1.21420	1.16508

Both software codes ran the exact same 24 input decks for both the HMF-001 and HMF-004 models, for all the iterations, (30%, 20%, 10%, 5%, 1%, 0.5%, 0.1%, 0.05%, and 0.01%).

Tables 11 and 12 contains the data from MCNP6 and MCNPX respectively.

The two tables are arranged from top to bottom by increasing iteration values. The first column displays the file extensions, as a reference. The second and third column display the nomenclature and perturbed iteration. The fourth and fifth columns are for the MT1-MT4 perturbed MCNP6 runs, while the sixth and seventh columns are for the MT1-MT4/MT18-MT38 perturbed MCNP6 runs.

The first six lines of both tables indicate a zero percent perturbing of the compared cross-sections, calculations, and experiments. This allow a direct analysis of the ENDF/B-V cross-sections, ENDF/B-VII cross-sections, previous MCNP6 calculations, baseline cross-sections, and the actual experiment values for both of the models HMF-001 and HMF-004. Remember that the model HMF-001 is a bare-sphere and the HMF-004 is a water-reflected, bare-sphere. This results in a difference in the both the neutron spectrums and the K_{eff} . This is a deliberate consideration as a boundary condition for both comparison and contrast.

In the Tables 11 and 12 are the comparisons of the two models with only MT1-MT4 perturbed, and then MT1-MT4 (columns 4-5) and MT18-MT38 (columns 6-7) perturbed. The difference being that MT1-MT4 is the scattering component of the cross-sections, and the MT18-MT38 is the fission component of the cross-sections.

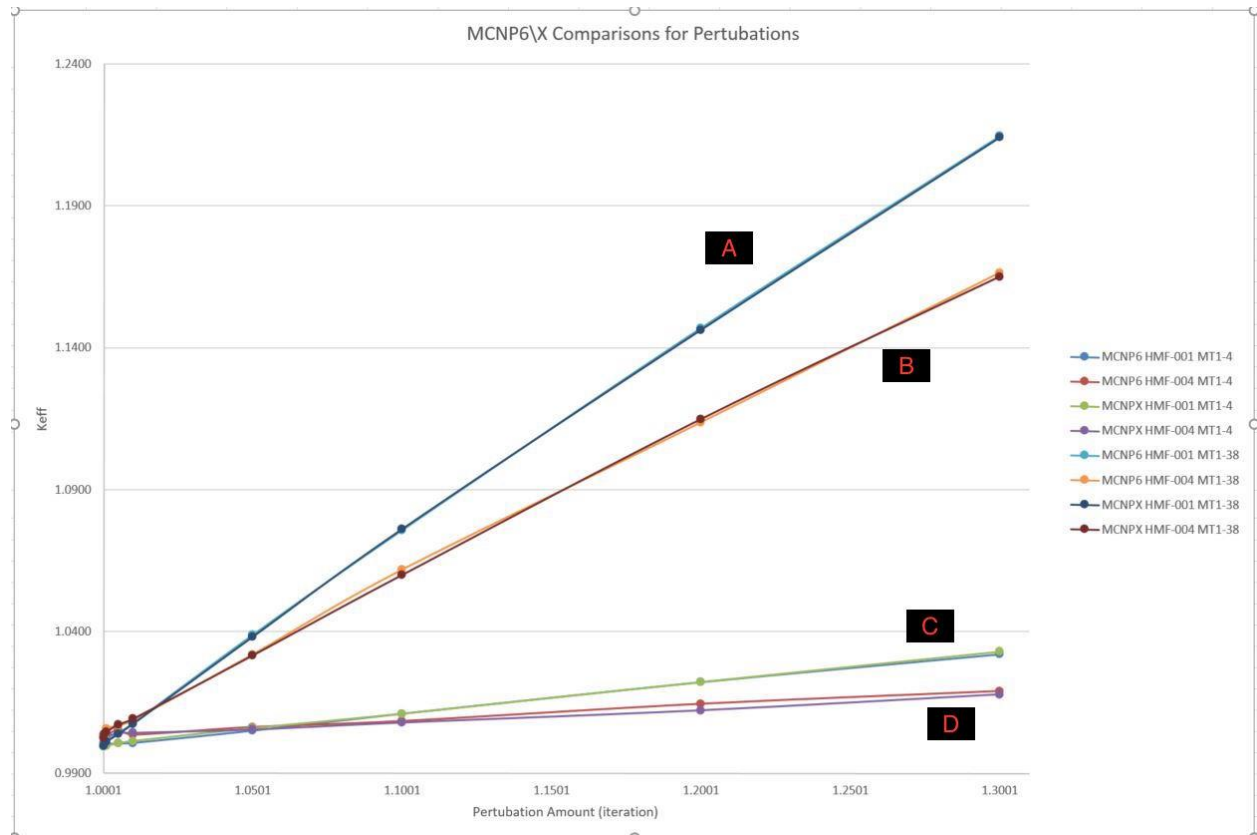
Table 13: Slopes of Perturbation Amount to Increase in K_{eff}

Slopes		MT1-4	MT1-4		MT18-38		MT1-38	MT1-38
HMF-001	rise	0.02697	0.10788	15.3%	0.59544	84.7%	0.17583	0.70332
	run	25.00000	per % inc		per % inc		25.0000	per % inc
HMF-004	rise	0.01269	0.05076	9.4%	0.48764	90.6%	0.13460	0.53840
	run	25.00000	per % inc		per % inc		25.0000	per % inc

There is a clear indication of increasing K_{eff} with an increase in perturbing amount. Both MT1-MT4 and MT18-MT38 sections have a positive effect on K_{eff} , due to the broadening of the cross-sections. It is clear that perturbing the scattering cross-section had less of an effect on the increase in K_{eff} , than perturbing the fission cross-sections.

In Figure 14, the comparisons of the two sets of Monte Carlo codes are displayed, using columns 3-7 of both Table 11 and 12. The increases in K_{eff} are linear with the increase in incremental perturbing of the cross-sections, as shown above in Table 13. The eight lines represent the two models of HMF-001 and HMF-004, the two codes MCNP6 and MCNPX, and the two comparisons of MT1-MT4 versus MT1-MT4/MT18-MT38.

Figure 14: MCNP6/X Comparisons for Perturbations



The uppermost lines (referred to as Group A curves) in Figure 14 are the MCNP6 and

MCNPX lines for the HMF-001 model, with both the MT1-MT4/MT18-MT38 sections perturbed. The second uppermost lines (referred to as Group B curves) in Figure 14 are the MCNP6 and MCNPX lines for the HMF-004 model, again with both the MT1-MT4/MT18-MT38 sections perturbed. The second lowermost lines (referred to as Group C curves) in Figure 14 are the MCNP6 and MCNPX lines for the HMF-001 model, with only the MT1-MT4 sections perturbed. The lowermost lines (referred to as Group D curves) in Figure 14 are the MCNP6 and MCNPX lines for the HMF-004 model, again with only the MT1-MT4 sections perturbed.

Figure 15: Neutron Facts from HMF-001 and HMF-004 at +30%

HMF-001	perturbed	Keff	ave E fission	Lethargy	Nu	pct (%) fission from neutrons		
MCNP6	amount		MeV			<0.625eV	inter	>100keV
*.50c	1	0.99761	1.5696	0.95636	2.607	0	3.51	96.49
*.86c	1	0.99988	1.4606	0.82110	2.599	0	5.28	94.72
*.70c	1	1.00006	1.4592	0.82008	2.599	0	5.31	94.69
*.77c	1.0001	1.00083	1.4586	0.81998	2.599	0	5.31	94.69
*.76c	1.0005	1.00071	1.4584	0.81983	2.599	0	5.34	94.66
*.75c	1.001	1.00145	1.4582	0.82015	2.599	0	5.32	94.68
*.74c	1.005	1.00419	1.4583	0.82027	2.599	0	5.31	94.69
*.73c	1.01	1.00767	1.4594	0.82115	2.599	0	5.31	94.69
*.72c	1.05	1.03880	1.4617	0.82321	2.599	0	5.26	94.74
*.71c	1.1	1.07573	1.4640	0.82677	2.599	0	5.19	94.81
*.78c	1.2	1.14667	1.4726	0.83520	2.6	0	5.06	94.94
*.79c	1.3	1.21463	1.4792	0.84206	2.601	0	4.97	95.03

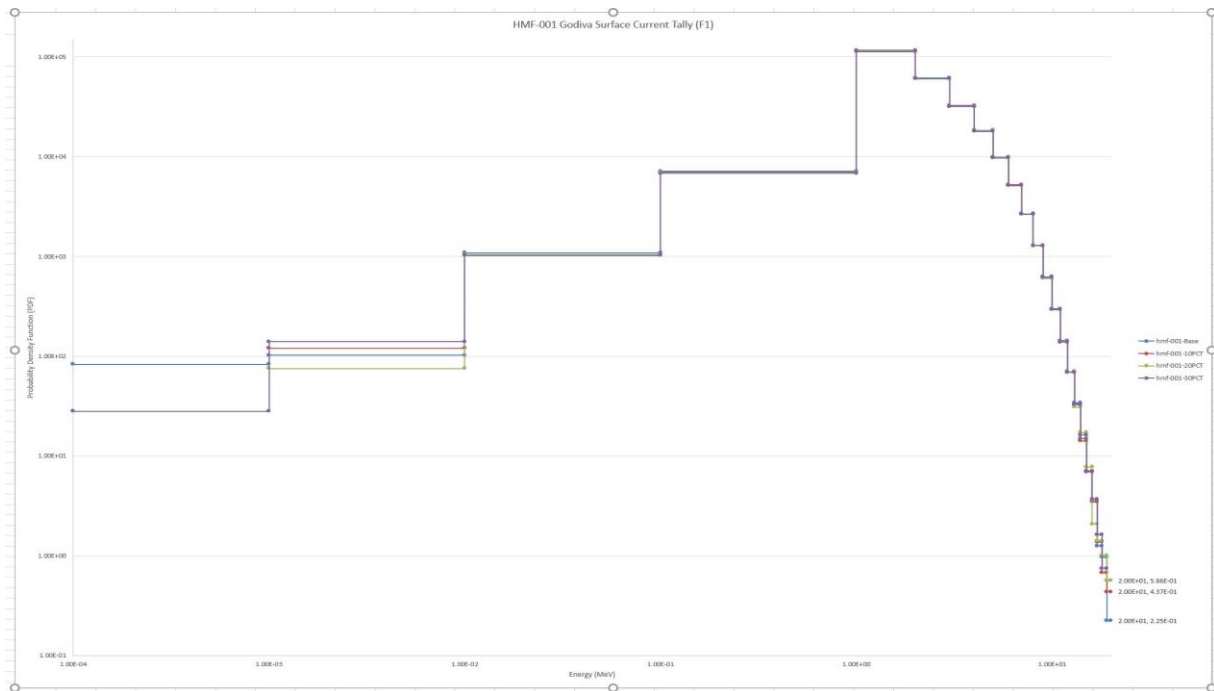
HMF-004	perturbed	Keff	ave E fission	Lethargy	Nu	pct (%) fission from neutrons		
MCNP6	amount		MeV			<0.625eV	inter	>100keV
*.50c	1	0.99734	1.1732	0.033020	2.564	14.56	14.43	71.01
*.86c	1	1.0035	1.0927	0.026841	2.558	15.09	15.78	69.13
*.70c	1	1.00416	1.0930	0.027281	2.558	14.98	15.80	69.21
*.77c	1.0001	1.00286	1.0913	0.027067	2.557	15.05	15.80	69.16
*.76c	1.0005	1.00341	1.0925	0.027487	2.558	14.96	15.77	69.27
*.75c	1.001	1.00583	1.0928	0.027442	2.558	14.94	15.83	69.23
*.74c	1.005	1.00678	1.0926	0.027597	2.557	14.91	15.82	69.27
*.73c	1.01	1.00883	1.0953	0.028015	2.558	14.82	15.80	69.38
*.72c	1.05	1.03192	1.1139	0.032054	2.560	14.28	15.33	70.40
*.71c	1.1	1.0618	1.1310	0.036844	2.562	13.72	14.87	71.42
*.78c	1.2	1.11373	1.1662	0.049294	2.566	12.43	14.02	73.54
*.79c	1.3	1.16652	1.2001	0.061791	2.570	11.50	13.22	75.28

Evaluating the graph with the six-factor formula, will shed some light on the reasons why

the curves in the graph are shaped the way they are. The HMF-001 bare-sphere model (Group Curves A and C) produces about 95% of the fissions in the >100 keV energy range, and about 5% in the >0.625 eV to <100 keV energy range, as seen in Figure 15. This greatly simplifies the equation for HMF-001 calculations, because the majority of the fissions are in the fast spectrum.

As the perturbing iteration incremental increases, the spectrum gets just a slight bit harder. As seen in Figure 15, the percent fission from neutrons only changes a few tenths of a percent to favor the >100 keV column.

Figure 16: Neutron Spectrum in HMF-001

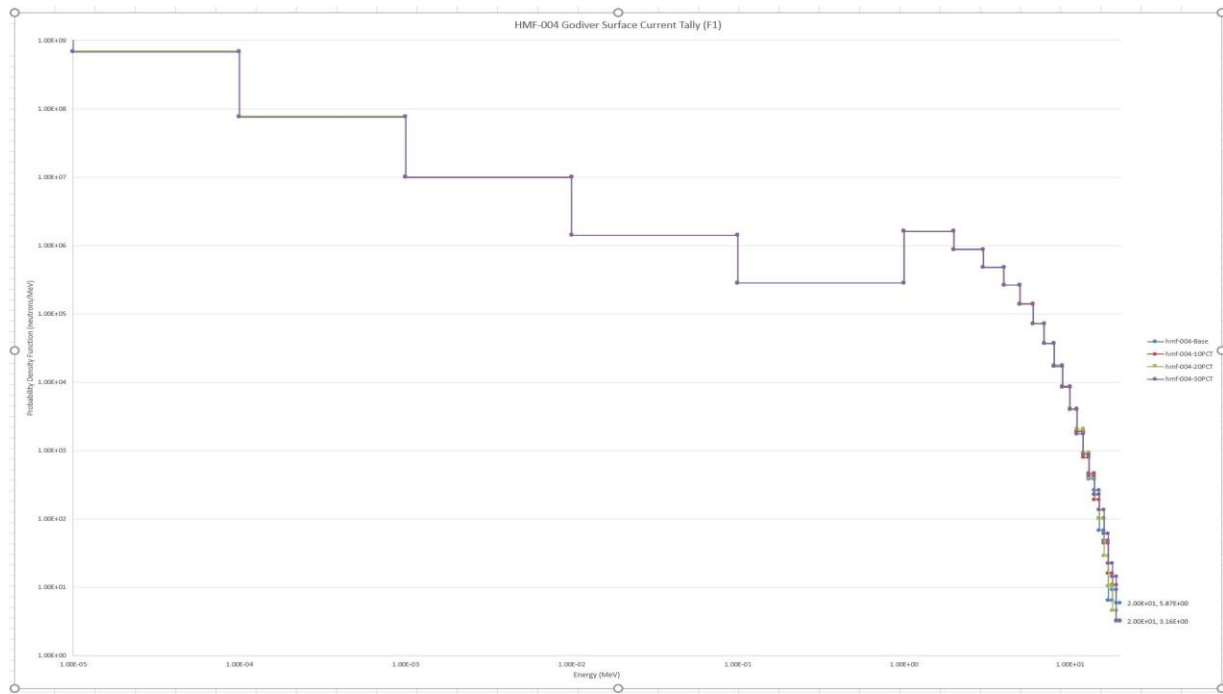


The HMF-004 model (Group Curves B and D) is about 15% for <0.625 eV, about 15% for >0.625 eV to <100 KeV, and about 70% for the >100 keV range. This is a softer or more thermal spectrum for the water-reflected HMF-004 model.

Figure 16 and 17 give a visual indication of the neutron spectrum from the HMF-001 and

HMF-004 models in MCNP6. The spectrums are similar for the MCNPX runs.

Figure 17: Neutron Spectrum in HMF-004



It is apparent that only a slight change in neutron population will make large changes in the K_{eff} . Neutron flux is a tightly calculated and controlled design parameter, due to the effect on the neutron life cycle and the direct effect on fuel consumption. Understanding those changes are important and finding the correct balance between geometry, poisons, and fuel loading are all important factors for any type of component.

The neutron life cycle is approximated by the six-factor formula. The variable K_{eff} is the product of the formula and it is equal to terms of L_f , ρ , L_{th} , f , η , and ϵ multiplied together.

In analyzing the HMF-001 model first (Group A curves), the majority of the fissions are in the fast energy region, so the thermal terms can “effectively” fall away, meaning ρ , L_{th} and f

can drop out of the equation. The reproduction factor does not largely change, as evidenced by Figure 15 column 6, because ν stays the same, (~ 2.599), but the change in the scattering cross-sections will have a minor impact on η . This results in an effective and usable equation of $K_{eff} = L_f * \epsilon * \eta$.

The L_f term decreases, due to the increase in population of fast neutrons not escaping, because of the contribution of MT1-MT4 values are increasing. This effect is because while the scattering cross-sections have increased, the neutrons are being reflected out of the sphere as well as back into the sphere. The net effect is a slight increase in K_{eff} from the scattering back into the sphere.

As seen in Table 13, about 15.3% of the change in K_{eff} , comes from perturbing the scattering cross-sections, (MT1-MT4), while 84.7% of the increase in K_{eff} comes from perturbing the fission cross-sections, (MT18-MT38). The fast fission factor (ϵ) is the strongest variable in this situation, and governs the K_{eff} value to increase overall.

In analyzing the HMF-004 model (Group B curves), a large majority of the fissions are in the fast energy region, but there is almost 30% of the fissions are in the <100 keV energy region. This means that the water-reflected sphere provides a contribution to the thermal terms in the six-factor formula, and they cannot drop out. A matter to note from Figure 15 is that the contribution to the amount of fissions from the lower two energy ranges, <100 keV, decreases about 5% while the >100 keV range increase by the same amount. This indicates a hardening of the neutron spectrum and less thermal fissions occurring.

Increasing the scattering cross-sections of the neutrons increases the probability of radiative capture in the resonance energy range, and thus increasing p and f . The reproduction factor still does not largely change, as evidenced by Figure 15 column 6, because ν stays the

same, (~ 2.555). The change in the scattering cross-sections will have a minor impact on η .

The L_f and L_{th} terms decrease, due to the increase in population of fast neutrons not escaping, because of the contribution of MT1-MT4 values are increasing. This effect is because while the scattering cross-sections have increased, the neutrons are being reflected out of the sphere as well as back into the sphere by the water. The net effect is a slight increase in K_{eff} from the scattering back into the sphere.

As seen in Table 13, about 9.4% of the change in K_{eff} , comes from perturbing the scattering cross-sections, (MT1-MT4). This is a decrease in 5% from that HMF-001 model. This indicates that the increase in thermal cross-sections have a strong effect on K_{eff} , slightly over the scattering cross-sections. The fast fission factor (ϵ) is still the strongest variable in this situation, and governs the K_{eff} value to increase overall, because of 90.6% of the increase in K_{eff} still comes from perturbing the fission cross-sections and 75% of the fissions from fast neutrons, (MT18-MT38).

In analyzing the HMF-001 model again (Group C curves), the majority of the fissions are in the fast energy region, so the thermal terms can again “effectively” fall away, meaning ρ , L_{th} and f can drop out of the equation. The reproduction factor does not largely change, as evidenced by Figure 15 column 6, because ν stays the same, but the change in the scattering cross-sections will have a larger impact on η . This results in the equation of $K_{eff} = L_f * \epsilon * \eta$.

The L_f term decreases, due to the increase in population of fast neutrons not escaping, because of the contribution of MT1-MT4 values are increasing. This effect is because while the scattering cross-sections have increased, the neutrons are being reflected out of the sphere as well as back into the sphere. The net effect is a slight increase in K_{eff} from the scattering back into the sphere.

As seen in Figure 14 and Table 13, an increase of 1% of the baseline K_{eff} has occurred from just perturbing the scattering cross-sections every 10%, (MT1-MT4). This is a much smaller increase in the K_{eff} versus perturbing both the fission and scattering cross-sections.

In analyzing the HMF-004 model (Group D curves), a large majority of the fissions are in the fast energy region, but there is still about 30% of the fissions are in the <100 keV energy region. This means that the water-reflected sphere provides the contribution to the thermal terms in the six-factor formula, and they do not drop out. A matter to note from Figure 15 is that the contribution to the amount of fissions from the lower two energy ranges, <100keV, still decreases about 5% while the >100keV range increase by the same amount when increasing the perturbing cross-sections from 0-30%. This indicates a hardening of the neutron spectrum and less thermal fissions occurring, due to more capture and leakage.

The newly created Fortran code perturbed the cross-sections successfully, from 0.0001 to 0.3, in minor increments. The Monte Carlo calculations used the perturbed cross-sections to verify that the changes in the cross-sections would produce changes in the K_{eff} . This also was positively accomplished.

After reviewing the K_{eff} versus perturbing amounts, from Table 11 and Table 12, the indicated amount perturbing before an indication of a change in K_{eff} is about 0.001. While this seems small, the cross-sections are typically 5 to six decimal places in accuracy.

CHAPTER 5: SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

Perturbing the cross-sections was to be able to show that the cross-section's sensitivity was linearly proportional to the amount of the perturbation above the amount of 0.001. This was easily demonstrated using MCNP6. The MCNPX runs paralleled the trends, but the numbers were a bit different. Determining the sensitivity to which the effect on K_{eff} changes is the end result of this study.

The calculations showed that if the scattering cross-sections were only perturbed, then a 10% increase in values in the MT1-MT4 sections produced a 1% increase in K_{eff} . If the fission and scattering cross-sections were perturbed, then a 10% increase in values in the MT1-MT4 and the MT18-MT38 sections produced a 6% increase in K_{eff} . This was using the HMF-001 model. This means that if only the MT18-MT38 sections were perturbed, then a 5% increase in K_{eff} is the result. These increases in K_{eff} is most evident after the 0.001 perturbed increment.

Further cross-section work is always a benefit to the scientific community, and should be pursued as much as funding will provide. This level of sensitivity can be greatly improved with additional experiments to improve the breadth and depth in knowledge of the isotopes of concern. U-234, U-235, U-236, and U-238 were selected from all the isotopes because of the large amount of work conducted by the reactor, weapons and research industries. These are well-known isotopes, but they still have sections of the cross-sections that are not as well defined as other sections. Appendix L displays the evolution of U-235 and U-238 from ENDF/B-V through NDF/B-VII.1 by shades of grey in gradient. Peaks get more definition and resonance range data expands. This work needs to continue to fill out the unresolved resonance range area.

Referring to Table 8, all of the isotopes of concern do not have the same amount of energy pairs as the others. This alone shows that there should be additional research to find those

pairs and then to determine the sensitivity of the pairs. Resonance regions improvements are very important, and can be documented better with more cross-section experiments, but that analysis is a topic for follow-on doctoral candidates.

Producing professional software that can streamline the Fortran95 code and combine it with the NJOY software would also be a good research topic. This will provide for better transitions from unprocessed ENDF files to modified ENDF files.

Future research requires comprehension of the entire structure of the ENDF files, including the subparts. The changes to the ENDF file quality will only come if a demand signal is generated from the users of the cross-sections. Better coordination of the quality and format of the cross-sections is required so all sections of the ENDF file can be used correctly. Uncertainty has been incorporated into the ENDF file structure as MT31-33, perhaps sensitivity can be added in the future as well...maybe as MT35?


APPENDIX A: ENDF FILE FORMATTING

Comparison of U-234, U-235, U-236, and U-238 ENDF formatting

		ENDF FILE CONTENTS FOR NLBO (NSUB/MF/MT)				NSUB Comments	MF Comments
		U234's MT	U235's MT	U236's MT	U238's MT	Photonuclear Data	
NSUB=0							
	MF1	451, 456	452, 455, 456	456	452, 455, 456		General Description
	MF3	3,5,16,18	3,5,16,18	3,5,16,18	3,5,16,17,18		fission Cross Section
	MF4	5,16,18	18	5,16,18	18		Angle distro
	MF5	5,16,18	18,455	5,16,18	18,455		Energy distro
	MF6		5,16		5,16,17		Product Angle and Energy distro
NSUB=4						Decay	
	MF1	452	452	452	452		
	MF8	457	457	457	457		
NSUB=5						Spontaneous FPY	
	MF8				454, 459		Decay Data
NSUB=10						Neutron	
	MF1	452, 455, 456	452, 455, 456, 458	452, 455, 456	452, 455, 456		General Description
	MF2	151	151	151	151		Resonances
	MF3	1,2,3,4,16-21,37,38,51-91,102	1,2,3,4,16-21,37,38,51-91,102	1,2,3,4,16-21,37,38,51-91,102	1,2,3,4,16-21,37,38,51-91,102		fission cross section
	MF4	2,18-21,38,51-90	2,18,51-90	2,18-21,38,51-90	2,18,51-90		Angle distro
	MF5	18-21,38,455	18,455	18-21,38,455	18,455		Energy distro
	MF6	16,17,37,91	16,17,37,91	16,17,37,91	16,17,37,91		Product Angle and Energy distro
	MF8	16,17,102	16,17,102	16,17,102	16,17,102		Decay Data
	MF12	18,102	4,18,102,460	18,102	18,102		photon production multiplicities
	MF13	3	3	3	3		photon production XS
	MF14	3,18,102	3,4,18,102,460	3,18,102	3,18,102		photon angular distro
	MF15	3,18,102	3,18,102	3,18,102	3,18,102		Continuous photon energy spectra
	MF31	456	452, 456	456	452, 456		Covariances of average neutrons per fission
	MF33	2,4,16,18,102	1, 2, 4, 16, 17, 18, 102	2,4,16,18,102	1, 2, 4, 16, 17, 18, 102		Covariances of neutrons cross-sections
	MF35		18		18		Covariances of energy distro of 2nd particles
NSUB=11						neutron induced FPY	
	MF8	454,459	454,459	454,459	454,459		Decay Data
NSUB19						Standard	
	MF3		18		18		fission cross section
	MF33		18		18		covariance cross sections

APPENDIX B: NJOY LICENSE

Copy of the License for NJOY 2012

 Los Alamos NATIONAL LABORATORY	MAIL TO: Los Alamos National Laboratory Attention: Richard P. Feynman Center for Innovation P.O. Box 1663, MS P 245 Los Alamos, NM 87545 Email: cmt-tt@lanl.gov Phone (505) 665-6707 Fax (505) 665-0154
Date: 9/17/2015 Invoice Number: 2015-611	
PLEASE MAKE CHECKS PAYABLE TO "Los Alamos National Laboratory"	

To:	Technology Description:
Lawrence Lakeotes, UNLV Advanced Doctoral Candidate 3128 Winter Sunset Ave North Las Vegas, NV 89081	NJOY2010_NJOY2012

Only the terms and conditions of the above referenced contract are accepted.

Agreement #	Type of Agreement	Purchase Order #
15-N03677	License	

Title	Description	Amount Due
Issue Fee	Nonrefundable License Issue Fee due and payable upon execution of End User License Agreement 15-N03677	\$500.00
	Total Due:	\$500.00

DUE: 11/2/2015
To ensure proper application of your payment, please identify LANL's agreement # in your remittance.
Checks: Payable to "Los Alamos National Laboratory" see "MAIL TO:" address above.
Wire Transfer: Wells Fargo Bank, 550 California (10), San Francisco, CA 94104 Routing #: 121000248 (ABA Number) Account #: 4121313753 (Los Alamos National Laboratory) SWIFT Code: WFBUS6SSFO
Express Mail Address: Los Alamos National Laboratory Bikini Atoll Rd. SM 30 Los Alamos, NM 87545
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Thank you for working with Los Alamos National Laboratory

APPENDIX C: MCNP6/X LICENSE

Copy of the License Approval for MCNP6/MCNPX

University of Nevada, Las Vegas Mail - RSICC Request Status

Page 1 of 3



Lawrence Lakeotes <lakeotes@unlv.nevada.edu>

RSICC Request Status

3 messages

RSIC <rsic@ornl.gov>

Thu, Aug 15, 2013 at 5:30 PM

To: "lakeotes@unlv.nevada.edu" <lakeotes@unlv.nevada.edu>

Dear Mr. Lakeotes,

All of the necessary approvals have now been received and the **MCNP6.1/MCNP5/MCNPX-EXE C810MNYCP01** software will be provided to you under the terms of the Single User Software License and Software Export Control Agreement forms you signed and submitted in addition to the stated conditions from ORNL's Office of Export Control below.

RSICC software codes are provided for RSICC Approved Users ONLY. The Approved User must not share software with others and the Approved User does not have permission to export the codes or documentation and should protect the software, documentation, and installation accordingly. Approved Users CAN NOT post RSICC software or manuals to the internet. In addition, the RSICC License prohibits the software licensee from allowing other individuals or entities to use the software. The RSICC Software Export Control Agreement obligates each software licensee to abide by all export control laws and regulations (No Exceptions). This includes preventing access to the software by any individual or entity (including system administrators) if such access may be deemed an export control violation.

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Thank you for your business,

Teresa Maave, RSICC

Oak Ridge National Laboratory

Reactor and Nuclear Systems Division

PO Box 2008

Oak Ridge TN 37831-6003

865-574-6176

<https://mail.google.com/mail/u/1/?ui=2&ik=614a0611a9&view=pt&q=rsicc&qs=true&sea...> 1/21/2016

APPENDIX D: ENDF_MODIFY CODE

Copy of the Fortran 95 ENDF Modify Code

```

C23456789012345678901234567890123456789012345678901234567890123456789012
C      1      2      3      4      5      6      7
C
C      PROGRAM ENDF_MODIFY ; PARAMETER (VERSION = 1.06) ; ! TYPE : F77
C      SYSTEM : INDEPENDENT DATE : JAN,2016 CLASS : UNCLASSIFIED
C      PROGRAMMER : L. LAKEOTES (UNLV/ME/PhD)
C
C      -----
C      |
C      |
C      |          C O D E - E N D F _ M O D I F Y . F O R
C      |
C      |          LAWRENCE LAKEOTES
C      |
C      | ENDF_MODIFY.FOR IS A PROGRAM FOR MODIFYING THE ENDF NUCLEAR
C      | CROSS SECTIONS. THE MODIFIED CROSS SECTIONS WILL BE USED FOR
C      | PERFORMING SENSITIVITY / PERTURBATION CALCULATIONS WITH THE
C      | BOLTZMANN TRANSPORT CODE: MCNPX.
C      |
C      | ENDF_MODIFY PERFORMES THE FOLLOWING 3 TASKS:
C      | 1) READ ENDF X-SECTIONS FROM THE ORIGINAL ENDF DATA FILES
C      | 2) MODIFIES ONLY SELECTED xS (REGION-OF-INTEREST ONLY)
C      |   - Xs ENERGY VALUES ARE NOT ALTERED
C      |   - ROI Xs ARE MULTIPLIED BY A FACTOR OF 1.1NN IN THE NSUB5
C      |     8, 10, AND 11 PORTIONS OF U234, U235 AND U238 ISOTOPES
C      |     (MULTI-FACTORS = 1.00, 1.05, 1.10, 1.15, 1.20, & 1.50)
C      | 3) WRITE THE PERTURBED Xs INTO NEW (MODIFIED) ENDF DAT FILES
C      |   - PERTURBED Xs WILL BE GENERATED FOR U234, U235 AND U238
C      |
C      |
C      | CODE MODIFICATIONS
C      | -----
C      |
C      | Ver  Mods  Description
C      | 1.00  LL   Insert subroutines
C      | 1.01  LCS   Add read & write features
C      | 1.02  LL   Modify write formation specifications
C      | 1.03  LCS   Correct columns
C      | 1.04  LL   Modify code to coreect output
C      | 1.05  LL   Correct multipliers
C      | 1.06  LL   Correct minor issues
C      |
C      | WARNIER-ORR DIAGRAM
C      | -----
C      |
C      | MAIN ---+
C      | PROGRAM |
C      |         +--- SUBROUTINE HEADINGS
C      |         |
C      |         +--- SUBROUTINE MAKE_MASTER_TABLE (Option #1)
C      |         |
C      |         +--- SUBROUTINE GEN_ENDF_MODIFY (Option #2)
C      |         |
C      |         | +--- SUBROUTINE SUB_ENDF_MODIFY
C      |         | |
C      |         | +--- SUBROUTINE READ_FILEINFO
C      |         |
C      |         +--- SUBROUTINE SUB_ENDF_MODIFY (Option #3)
C      |         |
C      |         +--- SUBROUTINE READ_FILEINFO

```

```

C |
C |      +-- SUBROUTINE MAKE_DEMO      (Option #4)
C |
C |
C |
C |-----
C
C
C
C
C PROGRAMMER'S NOTES
C =====
C
C BASIC FORTRAN RULES
C -----
C Columns for Standard F77
C   C - Col #1      - Comment
C   ! - any Col     - Rest of line is a Comment
C   ; - any Col     - Rest of line is a New Line
C   - Col #1 -> #5   - Fortran Statement Number
C   + - Col #6      - Any standard non-zero character =continuation
C   - Col #7 -> #72 - FORTRAN-77 statements
C   - Col #73-> #80 - Sequential Identification Numbers
C
C Default Names for Variables & Function Subprograms
C   A -> H   &   O -> Z   - are reals           I -> N   - are INtegers
C
C I/O Logical Units
C   5 - standard input (or from screen)
C   6 - standard output (or to screen)
C  11-19 - recommended LUs for input files
C  21-29 - recommended LUs for output files
C
C Operations
C   IF( .??. )   IF decision statement control
C   .GE. = greater than or equal   .EQ. = equals   .LT. = less than
C   .LE. = less than or equal     .OR. = or       .AND. = and
C   ENDIF      End a nested IF structure
C   DO 1000 I=a,b,c   = perform a nested do-loop, start at "a",
C                     end at "b", use increments of "c"
C 1000 CONTINUE
C
C Functions & Subroutines
C   X=AAA(a,b,...)      execute function AAA, input variables are in
C                       parenthesis, AAA is output +exchange (a,b...
C   CALL BBB(a,b,c,d,...) call subroutine BBB, exchange (a,b,...
C
C Write Statement & Formats
C
C   WRITE(LU6,9010) A,B,C,I   - write "a,b,c,i" to device #6 (screen)
C 9010 FORMAT(T3,F9.0,5X,F8.1,/,3X,1P1E14.7,2X,I3)   - "T" - column,
C                                           "X" -spaces, "/" - new line, "$" - no new line
C
C   Integers      - Iw      w-width
C   Reals          - Fw.d   w-wide, d-digits after .
C                 - Ew.d -- E14.7 -scientific notation w=14, d=7
C   Real Extra    - sP1Ew.d -- 1P1E14.7 -- s=1 (scalar multiplier)
C
C Special
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)      ! Work in double precision
C   CHARACTER*200 LINE      ! Character string "LINE" (length=200)
C   LINE(1:LEN_TRIM(LINE))      ! Return length of "LINE"
C
C SUGGESTIONS
C -----
C   1) USE DEFAULT NAMING CONVECTION FOR INTEGERS & REALS
C   2) USE ALL UPPER CASE LETTERS
C   3) USE SIMPLE LOOP AND DECISION STRUCTURES
C   4) USE MANY COMMENT STATEMENT FOR DOCUMENTION

```

```
C      5) USE DOUBLE PRECISION AS THE DEFAULT FOR FLOATING-POINT VALUES
C
C
C
C
C _____ ENDF_MODIFY _____
C
C234567
C
C      PROGRAM MAIN
C
C      LU5=5   ;   LU6=6
C
C      CALL HEADINGS(VERSION)
C
C      WRITE(LU6,9100)
9100 FORMAT(
       1 /,T5,'[L2Q1] IDENTIFY WHICH TASK OPERATION TO PERFORM',
       2 /,T5,'          [1] MAKE MASTER TABLE',
       3 /,T5,'          [2] GENERATE NEW ENDF FILES (USING MASTER TABLE)',
       4 /,T5,'          [3] GENERATE A SINGLE "NEW" ENDF FILE (WITHOUT',
       5 /,T5,'              USING MASTER TABLE)',
       6 /,T5,'          [4] MAKE DEMO FILES',
       7 /,T5,'                                     <1> ', $)
8100 FORMAT(I1)
      IF(IOPTION.EQ.0) IOPTION=1
C
C      IF(IOPTION.EQ.1) CALL MAKE_MASTER_TABLE
C      IF(IOPTION.EQ.2) CALL GEN_ENDF_MOD_INP
C      IF(IOPTION.EQ.3) CALL SUB_ENDF_MODIFY
C      IF(IOPTION.EQ.4) CALL MAKE_DEMO
C
C      STOP
C      END
C
C
C
C      SUBROUTINE HEADINGS(VERSION)
C      THIS SUBROUTINE IS USED TO PRINT OUTPUT HEADINGS TO STANDARD OUTPUT.
C
C      REAL VERSION ; LU6=6
C
C      WRITE(LU6,9100) VERSION
9100 FORMAT(
       1 /,T5,70(' '),
       2 //,T27,'E N D F _ M O D I F Y',T60,'(VERSION:',F4.2,')',
       3 //,T29,'LAWRENCE LAKEOTES',
       4 /,T5,70(' '),//)
C
C      RETURN
C      END
C
C
C
C      SUBROUTINE MAKE_MASTER_TABLE
C      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C      THIS SUBROUTINE IS USED TO GENERATE A MASTER TABLE THAT LIST ALL THE
C      CROSS SECTIONS SETS TO BE GENERATED. THIS SUBROUTINE SHOULD BE
C      EXECUTED ONLY ONCE.
C      DOUBLE PRECISION XLM(100)
C      CHARACTER*200 Q1,Q2,Q3,Q4,Q5,CANS1,CANS2,CANS3,CANS4,CANS5
C      CHARACTER*4 C_NUCLIDE
C      LOGICAL EXT
C
C      LU5=5 ; LU6=6 ; LU21=21
C
C      WRITE(LU6,9000)
9000 FORMAT(
       1 /,T3,'EXECUTING "MASTER TABLE" CODE',
```

```

2 /)
C
  INQUIRE (FILE='MASTER_TABLE.DAT',EXIST=EXT)
  IF(EXT) THEN
    WRITE(LU6,9910)
9910  FORMAT(
1    //,T5,'<<ERROR>> -- FILE: "MASTER_TABLE.DAT" ALREADY EXIST -- ',
2    ' <<ERROR>>',
3    //,T5,'          PROGRAM EXECUTION HALTED'//)
    STOP
  ENDIF
C
  OPEN(LU21,FILE='MASTER_TABLE.DAT',STATUS='NEW')
  WRITE(LU21,9100)
9100  FORMAT(
1    //,T3,'LJL MASTER TABLE',
2    //,T3,'-----',
3    '-----',
4    /,T3,'Input Parameters          Computational Resul',
5    'ts',
6    /,T3,'Index      Linear ENDF_Lines',
7    ' ',
8    /,T3,'ID      Multip E_STR E_END Kinf Keff E>1 E>',
9    '10 E>100',
+   /,T3,'-----',
1   '-----')
C
  Q1='[Q1] ENTER ENDF NUCLIDE      {^C to Quit}      <'
  Q2='[Q2] ENTER ENDF DATA 1st ENERGY LINE START  <'
  Q3='[Q3] ENTER ENDF DATA 2nd ENERGY LINE START  <'
  Q4='[Q4] ENTER # OF ENERGY LINES TO BE CHANGED  ('
  Q5='[Q5] ENTER # OF Xs LINEAR MULTIPLIER VALUES  <'
C
  C_NUCLIDE='U234' ; LINE_STR=1000 ; LINE_END=1010
  LINE_DELTA=05 ; NUM_LM=2
C
1000  WRITE(LU6,"()")
      WRITE(LU6,9200) Q1(1:LEN_TRIM(Q1)),C_NUCLIDE(1:LEN_TRIM(C_NUCLIDE))
      READ(LU5,8100,END=5000) CANS1 ;
      IF(LEN_TRIM(CANS1).NE.0) C_NUCLIDE=CANS1(1:4)
      WRITE(LU6,9300) Q2(1:LEN_TRIM(Q2)),LINE_STR
      READ(LU5,8100) CANS2;IF(LEN_TRIM(CANS2).NE.0) READ(CANS2,*)LINE_STR
      WRITE(LU6,9300) Q3(1:LEN_TRIM(Q3)),LINE_END
      READ(LU5,8100) CANS3;IF(LEN_TRIM(CANS3).NE.0) READ(CANS3,*)LINE_END
      WRITE(LU6,9300) Q4(1:LEN_TRIM(Q4)),LINE_DELTA
      READ(LU5,8100) CANS4 ; IF(LEN_TRIM(CANS4).NE.0)
1     READ(CANS4,*)LINE_DELTA
      WRITE(LU6,9300) Q5(1:LEN_TRIM(Q5)),NUM_LM
      READ(LU5,8100) CANS5 ; IF(LEN_TRIM(CANS5).NE.0) READ(CANS5,*)NUM_LM
      DO 2000 I=1,NUM_LM
        WRITE(LU6,9400) (I+5),I,(1.00D0+0.05D0*DFLOAT(I))
        READ(LU5,9500) XLM(I)
        IF(XLM(I).EQ.0.0D0) XLM(I)=1.00D0+0.05D0*DFLOAT(I)
2000  CONTINUE
8100  FORMAT(A)
9200  FORMAT(T5,A,A,'> ',,$)
9300  FORMAT(T5,A,I4,'> ',,$)
9400  FORMAT(T7,'[Q',I2,'] ENTER Xs LINEAR MULTIPLIER #',I2,T53,'<',
1     F4.2,'> ',,$)
9500  FORMAT(F14.0)
C
  INDEX=0
  DO 4000 INUM=1,NUM_LM
    DO 3000 ISTR=LINE_STR,LINE_END
      INDEX=INDEX+1
      WRITE(LU21,9600) C_NUCLIDE,INDEX,XLM(INUM),ISTR,
1      (ISTR+LINE_DELTA-1)
9600  FORMAT(2X,A4,I5.5,2X,F5.2,3X,I6,1X,I6)
3000  CONTINUE
4000  CONTINUE
GO TO 1000

```

```
C
5000 CLOSE(LU21)
      RETURN
      END
C
C                                     -----|
C                                     | GEN_ENDF_MOD_INP |
C                                     !-----|
SUBROUTINE GEN_ENDF_MOD_INP
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
CHARACTER*80 LINE
CHARACTER*9 LABEL
LOGICAL EXT

C
LU6=6 ; LU11=11 ; LU21=21

C
C
C
INQUIRE(FILE='MASTER_TABLE.DAT',EXIST=EXT)
IF(.NOT.EXT) THEN
    WRITE(LU6,9910)
9910 FORMAT(
1 //,T5,'<<ERROR>>' -- FILE: "MASTER_TABLE.DAT" NOT FOUND -- ',
2 ' <<ERROR>>',
3 //,T5,' PROGRAM EXECUTION HALTED'//)
STOP
ENDIF

C
C
OPEN(LU11,FILE='MASTER_TABLE.DAT',STATUS='OLD')
READ(LU11,"(A)") (LINE,IDUMMY=1,10) ! READ/SKIP HEADER LINES

C
C
ICOUNT=0
1000 READ(LU11,"(A)",END=9991) LINE
      WRITE(LU6,9000)
9000 FORMAT(
1 T3,'EXECUTING "GEN_ENDF_MOD_INP" CODE -- XS file label: ', $)
READ(LINE,8100) LABEL,XLM,I_STR,I_END
8100 FORMAT(2X,A9,F7.0,2X,I7,I7)
      ICOUNT=ICOUNT+1
      OPEN(LU21,FILE='TMP_GEMI.TMP',STATUS='UNKNOWN')
      WRITE(LU21,9200) LABEL(1:4),LABEL,XLM,I_STR,I_END
9200 FORMAT('3',/,A4,'_MASTER.XS',/,A9,'_MOD.XS',/,F6.4,/,I6,/,I6)
      WRITE(LU6,9300) LABEL, ICOUNT
9300 FORMAT(A9,2X,'Icount=',I6)
      CLOSE(LU21)
      CALL SYSTEM("ENDF_MODIFY.EXE < TMP_GEMI.TMP") ! SYSTEM CALL
GO TO 1000

C
C
9991 CLOSE(LU11)
      STOP
      END
C
C                                     -----|
C                                     | SUB_ENDF_MODIFY |
C                                     !-----|
SUBROUTINE SUB_ENDF_MODIFY
C THIS SUBROUTINE IS USED TO MODIFY THE ENDF CROSS SECTION DATA FILES.
C IT WILL: READ THE DATA, MODIFY A SELECT SECTION, & REWRITE THE DATA.
C
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
CHARACTER*200 LINE,FILEOLD,FILENEW
LU6=6 ; LU11=11 ; LU21=21 ; ICOUNT=0
INPUT; READ; INPUT METHOD; OUTPUT METHOD;
CALL READ_FILEINFO(FILEOLD,FILENEW,LINE_START,LINE_END,XLM)

C
OPEN(LU11,FILE=FILEOLD,STATUS='OLD')
OPEN(LU21,FILE=FILENEW,STATUS='UNKNOWN')

C
C STAGE 01 - READ ENDF FILE HEADER DATA

DO 1000 I=1,(LINE_START-1),1
    READ(LU11,8100) LINE ; ICOUNT=ICOUNT+1
```



```

1                                READ(CANS5,*)L_END
C
9100 FORMAT(T7,A,T60,'<',A,'>', '$)
9110 FORMAT(T7,A,T61,'<',F5.3,'>', '$)
9120 FORMAT(T7,A,T60,'<',I6,'>', '$)
8100 FORMAT(A)
C
      WRITE(LU6,9130) F_IN(1:LEN_TRIM(F_IN)), F_OUT(1:LEN_TRIM(F_OUT)),
1 XLM, L_STR, L_END
9130 FORMAT(
1  /,T5,'USER INPUT STATISTICS',
2  /,T7,'INPUT FILE NAME = ',A,
3  /,T7,'OUTPUT FILE NAME = ',A,
4  /,T7,'LINEAR MULTIPLIER= ',F6.4,
4  /,T7,'ROI START LINE # =',I6,
5  /,T7,'ROI END   LINE # =',I6,
6  /)
C
      RETURN
      END
C
C                                -----|
C                                | MAKE_DEMO |
C                                !-----|
      SUBROUTINE MAKE_DEMO
C
C THIS SUBROUTINE IS USED TO MAKE DEMO INPUT FILES -- 1) A SCRIPT FILE,
C 2) AN INPUT FILE, AND 3) A DEMO MASTER XS (CROSS SECTION) FILE.
C
      LU21=21 ; LU22=22 ; LU23=23 ; LU24=24
C
      OPEN(LU21,FILE='TMP_DEMO_SCRIPT.BAT',STATUS='NEW')
      WRITE(LU21,9110)
9110 FORMAT(
1  '@REM -- DEMO SCRIPT FILE -- RUN EMDF_MODIFY',
2  /,'@ECHO.',
3  /,'@ECHO.',
4  /,'@ECHO. -- GENERATING DEMO FILES -- SCRIPT, INPUT, Xs',
5  /,'@ENDF_MODIFY.EXE < TMP_DEMO.INP1 > nul',
6  /,'@ECHO.',
7  /,'@ECHO.',
8  /,'@ECHO. -- GENERATE MASTER TABLE + INDIVIDUAL Xs FILES',
9  /,'@ENDF_MODIFY.EXE < TMP_DEMO.INP2 > nul')
      CLOSE(LU21)
C
C
      OPEN(LU22,FILE='TMP_DEMO.INP1',STATUS='NEW')
      WRITE(LU22,9210)
9210 FORMAT(
1  '1                <-- LEVEL #2 -- OPTION #1',
2  /,'TMP_          <-- NUCLIDE NAME (4 CHARACTERS)',
3  /,'11          <-- FIRST STARTING LINE FOR CHANGING XS (6 IN',
4  'TEGER DIGITS MAX)',
5  /,'13          <-- LAST  STARTING LINE FOR CHANGING XS (6 IN',
6  'TEGER DIGITS MAX)',
7  /,'3           <-- NUMBER OF LINES TO BE MODIFIED      (6 IN',
8  'TEGER DIGITS MAX)',
9  /,'4           <-- NUMBER OF LINEAR MULTIPLIERS          (6 IN',
+  'TEGER DIGITS MAX)',
1 /,'1.0         <-- 1ST LINEAR MULTIPLIER                (14 R',
2  'EAL DIGITS MAX)',
3 /,'1.07        <-- 2ND LINEAR MULTIPLIER                (14 R',
4  'EAL DIGITS MAX)',
5 /,'1.08        <-- 3rd LINEAR MULTIPLIER                (14 R',
6  'EAL DIGITS MAX)',
7 /,'2.00        <-- 4th LINEAR MULTIPLIER                (14 R',
8  'EAL DIGITS MAX)')
      CLOSE(LU22)
C
C
      OPEN(LU23,FILE='TMP_DEMO.INP2',STATUS='NEW')
      WRITE(LU23,9310)
9310 FORMAT(

```

```

1      '2          <-- LEVEL #2 -- OPTION #2')
      CLOSE (LU23)
C
C      OPEN (LU24, FILE='TMP__MASTER.XS', STATUS='NEW')
      WRITE (LU24, 9410)
9410  FORMAT ('12345678901234567890123456789012345678901234567890123456',
1      '7890123456')
      DO 4100 I=2,9
          WRITE (LU24, 9420)
9420  FORMAT ('TEST')
4100  CONTINUE
      DO 4200 I=10,20
          WRITE (LU24, 9430)
9430  FORMAT (' 1.234E+01 2.222E+02 3.333E+03 4.444E+04 5.555E+0',
1      '5 6.666E+06')
4200  CONTINUE
      DO 4300 I=21,30
          WRITE (LU24, 9420)
4300  CONTINUE
      CLOSE (LU24)
C
      RETURN
      END

```


APPENDIX E: NJOY2012 DOS BATCH FILE

NJOY DOS Batch File for U-234 for Baseline Cross-sections (*.70c). All other NJOY DOS Batch files are similar.

```
echo NJOY Dissertation Problem

echo getting endf from u234_nlib1_nsub10.txt
copy C:\NJOY2012\70C_base\u234\u234_nlib1_nsub10.txt
C:\NJOY2012\70C_base\u234\tape20

echo running njoy
c:\njoy2012\njoy<C:\NJOY2012\70C_base\u234\u234_base.dat

echo saving output
copy output C:\NJOY2012\70C_base\u234\u234_baseout.txt
copy tape29 C:\NJOY2012\70C_base\u234\92234.70c
copy tape30 C:\NJOY2012\70C_base\u234\u234_basexsdir.txt
copy tape59 C:\NJOY2012\70C_base\u234\u234_baseplot.ps
copy tape60 C:\NJOY2012\70C_base\u234\u234_basependf.txt
del tape20 tape21 tape22 tape23 tape24 tape25 tape26 output
del tape27 tape28 tape29 tape30 tape31 tape32 tape33
del tape34 tape59 tape60 fort.13
```

APPENDIX F: NJOY2012 DAT FILES

NJOY Input DAT File for U-234 for Baseline (*.70c)

```
moder
 20 -21
reconr
 -21 -22
 'U234 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
 9225 0 0/
 .001/
 0/
broadr
 -21 -22 -23
 9225 1 0 1 0/
 .001/
 300/
 0/
unresr
 -21 -23 -24
 9225 1 7 1 /
 300/
 1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
 0/
heatr
 -21 -24 -25 34/
 9225 12/
 302 303 304 318 401 402 442 443 444 445 446 447/
thermr
 0 -25 -26
 0 9225 16 1 1 1 1 1 221 2/
 300/
 .001 5/
gaspr
 -21 -26 -27
purr
 -21 -27 -28
 9225 1 7 20 4/
 300/
 1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
 0/
moder
-28 60
acer
 -21 -28 0 29 30
 1 0 1 .70 / U234 data at 300K
 'U234 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
 9225 300 '92234'/
 0/
 /
acer
 0 29 31 32 33
 7 1 1/
 'U234 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
viewr
 31 59/
stop
```

NJOY Input DAT File for U-235 for Baseline (*.70c)

```
moder
 20 -21
reconr
-21 -22
'U235 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
9228 0 0/
.001/
0/
broadr
-21 -22 -23
9228 1 0 1 0/
.001/
300/
0/
unresr
-21 -23 -24
9228 1 7 1 /
300/
1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
heatr
-21 -24 -25 34/
9228 12/
302 303 304 318 401 402 442 443 444 445 446 447/
thermr
0 -25 -26
0 9228 16 1 1 1 1 1 221 2/
300/
.001 5/
gaspr
-21 -26 -27
purr
-21 -27 -28
9228 1 7 20 4/
300/
1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
moder
-28 60
acer
-21 -28 0 29 30
1 0 1 .70 / U235 data at 300K
'U235 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
9228 300 '92235'/
0/
/
acer
0 29 31 32 33
7 1 1/
'U235 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
viewr
31 59/
stop
```

NJOY Input DAT File for U-236 for Baseline (*.70c)

```
moder
 20 -21
reconr
-21 -22
'U236 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
9231 0 0/
.001/
0/
broadr
-21 -22 -23
9231 1 0 1 0/
.001/
300/
0/
unresr
-21 -23 -24
9231 1 7 1 /
300/
1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
heatr
-21 -24 -25 34/
9231 12/
302 303 304 318 401 402 442 443 444 445 446 447/
thermr
0 -25 -26
0 9231 16 1 1 1 1 1 221 2/
300/
.001 5/
gaspr
-21 -26 -27
purr
-21 -27 -28
9231 1 7 20 4/
300/
1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
moder
-28 60
acer
-21 -28 0 29 30
1 0 1 .70 / U236 data at 300K
'U236 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
9231 300 '92236'/
0/
/
acer
0 29 31 32 33
7 1 1/
'U236 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
viewr
31 59/
stop
```

NJOY Input DAT File for U-238 for Baseline (*.70c)

```
moder
 20 -21
reconr
-21 -22
'U238 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
9237 0 0/
.001/
0/
broadr
-21 -22 -23
9237 1 0 1 0/
.001/
300/
0/
unresr
-21 -23 -24
9237 1 7 1 /
300/
1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
heatr
-21 -24 -25 34/
9237 12/
302 303 304 318 401 402 442 443 444 445 446 447/
thermr
0 -25 -26
0 9237 16 1 1 1 1 1 221 2/
300/
.001 5/
gaspr
-21 -26 -27
purr
-21 -27 -28
9237 1 7 20 4/
300/
1e10 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
moder
-28 60
acer
-21 -28 0 29 30
1 0 1 .70 / U238 data at 300K
'U238 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
9237 300 '92238'/
0/
/
acer
0 29 31 32 33
7 1 1/
'U238 Baseline from NNDC ENDF & NJOY2012.50 (ljlakeotes)'/
viewr
31 59/
stop
```

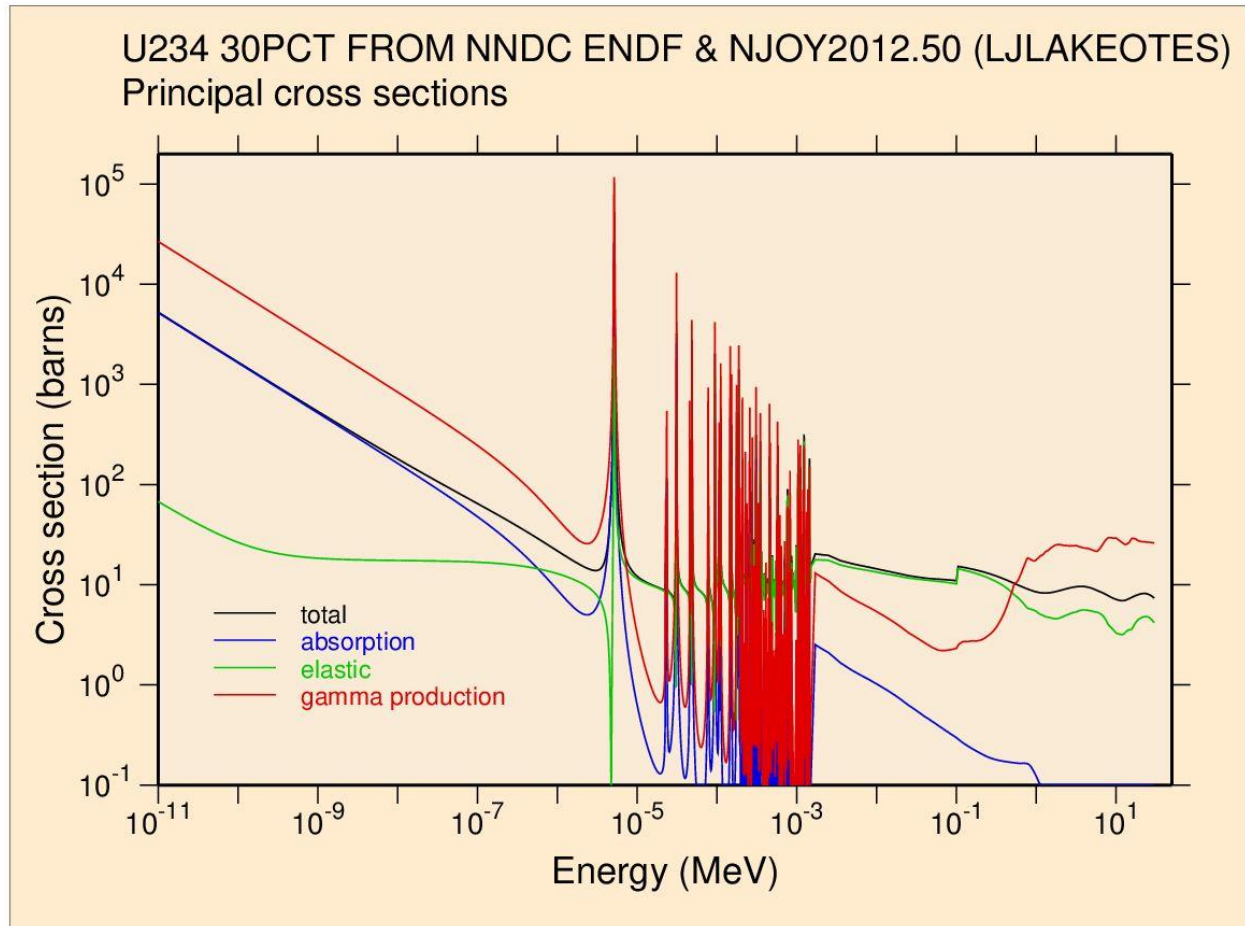
APPENDIX G: MASTER NJOY DOS BATCH FILE

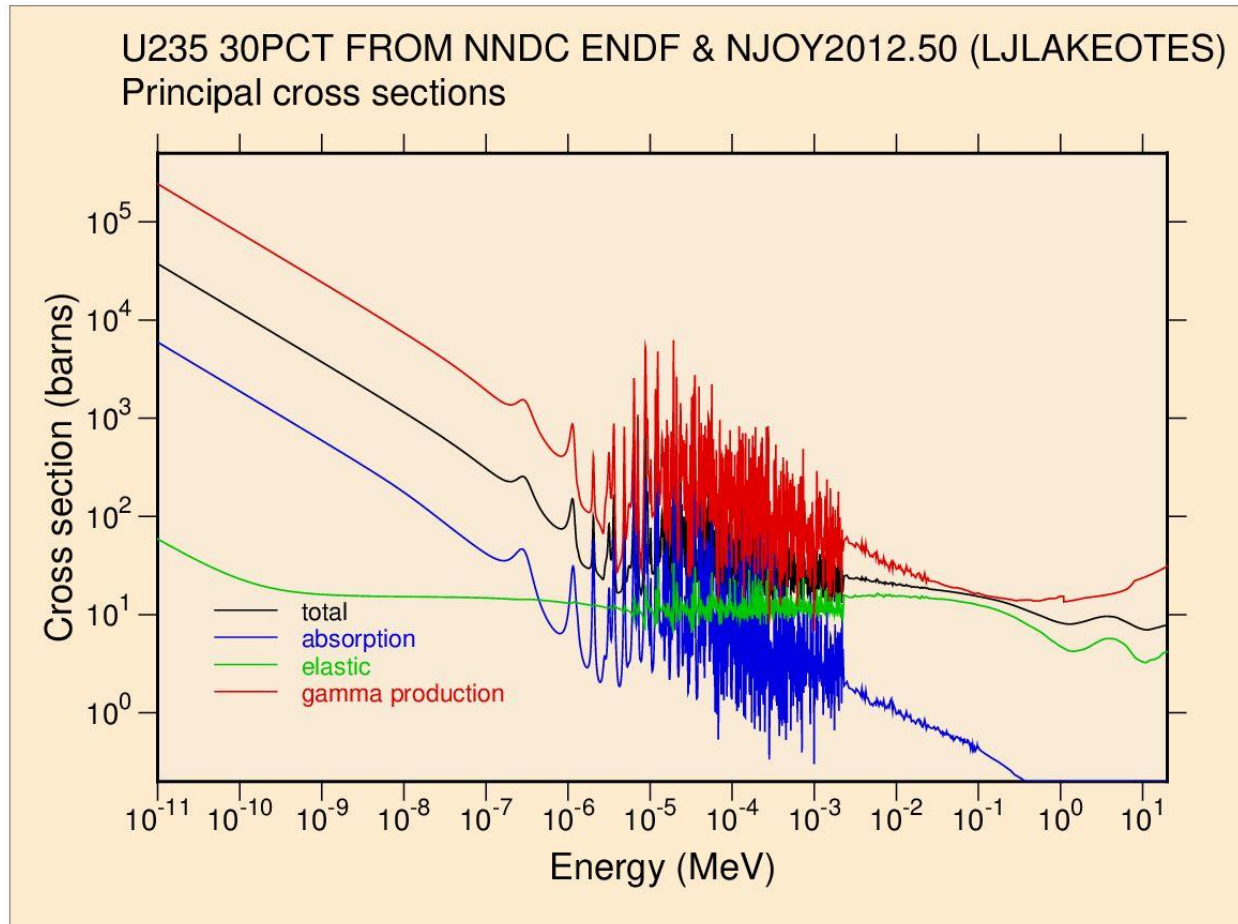
Master NJOY2012.50 DOS Batch File

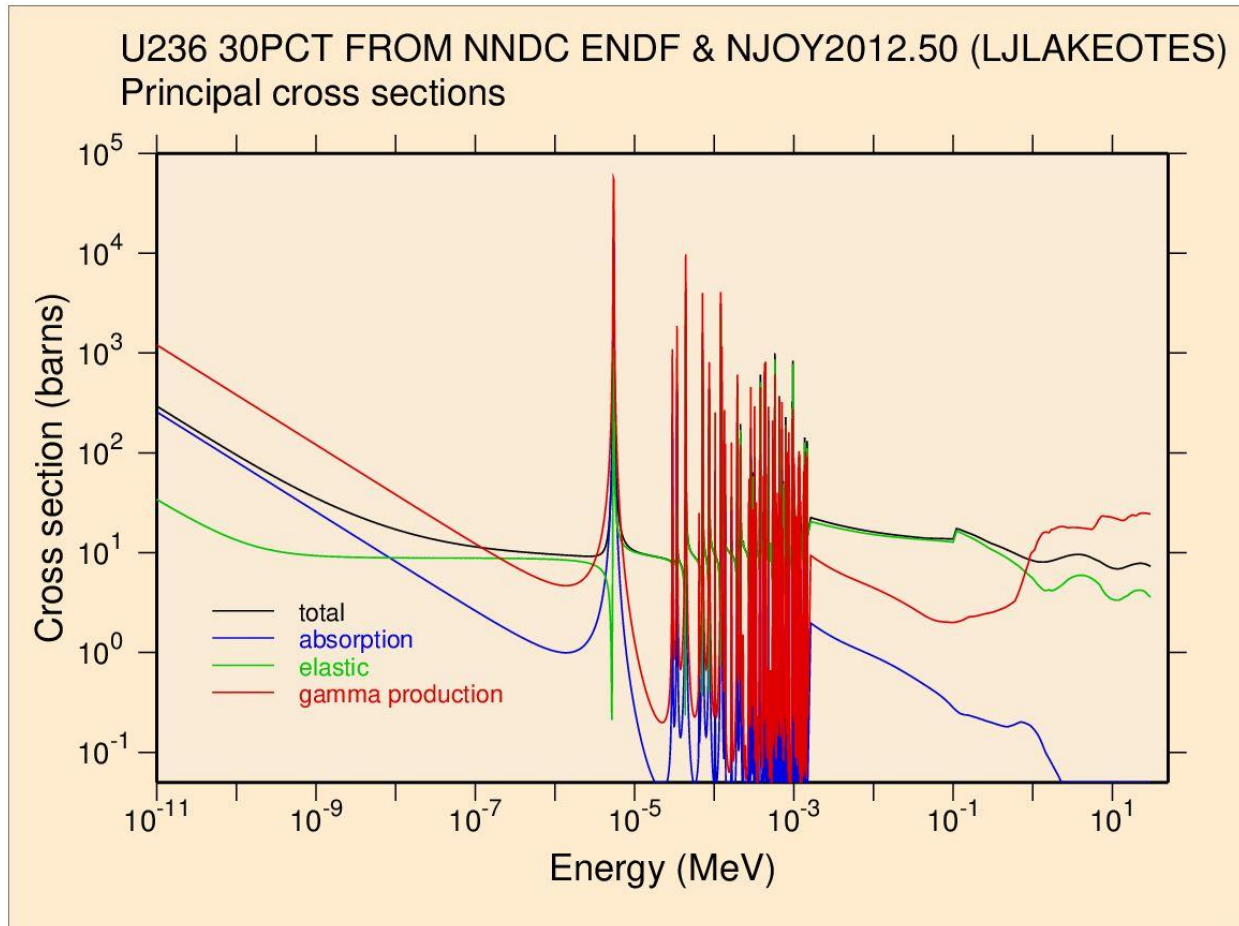
```
echo Master NJOY2012.50 DOS Batch File
echo one pertubation/isotope will be run at a time
C:\NJOY2012\70C_base\u234\u234_base.bat
C:\NJOY2012\70C_base\u235\u235_base.bat
C:\NJOY2012\70C_base\u236\u236_base.bat
C:\NJOY2012\70C_base\u238\u238_base.bat
C:\NJOY2012\71C_10PCT\u234\u234_10PCT.bat
C:\NJOY2012\71C_10PCT\u235\u235_10PCT.bat
C:\NJOY2012\71C_10PCT\u236\u236_10PCT.bat
C:\NJOY2012\71C_10PCT\u238\u238_10PCT.bat
C:\NJOY2012\72C_05PCT\u234\u234_05PCT.bat
C:\NJOY2012\72C_05PCT\u235\u235_05PCT.bat
C:\NJOY2012\72C_05PCT\u236\u236_05PCT.bat
C:\NJOY2012\72C_05PCT\u238\u238_05PCT.bat
C:\NJOY2012\73C_01PCT\u234\u234_01PCT.bat
C:\NJOY2012\73C_01PCT\u235\u235_01PCT.bat
C:\NJOY2012\73C_01PCT\u236\u236_01PCT.bat
C:\NJOY2012\73C_01PCT\u238\u238_01PCT.bat
C:\NJOY2012\74C_005PCT\u234\u234_005PCT.bat
C:\NJOY2012\74C_005PCT\u235\u235_005PCT.bat
C:\NJOY2012\74C_005PCT\u236\u236_005PCT.bat
C:\NJOY2012\74C_005PCT\u238\u238_005PCT.bat
C:\NJOY2012\75C_001PCT\u234\u234_001PCT.bat
C:\NJOY2012\75C_001PCT\u235\u235_001PCT.bat
C:\NJOY2012\75C_001PCT\u236\u236_001PCT.bat
C:\NJOY2012\75C_001PCT\u238\u238_001PCT.bat
C:\NJOY2012\76C_0005PCT\u234\u234_0005PCT.bat
C:\NJOY2012\76C_0005PCT\u235\u235_0005PCT.bat
C:\NJOY2012\76C_0005PCT\u236\u236_0005PCT.bat
C:\NJOY2012\76C_0005PCT\u238\u238_0005PCT.bat
C:\NJOY2012\77C_0001PCT\u234\u234_0001PCT.bat
C:\NJOY2012\77C_0001PCT\u235\u235_0001PCT.bat
C:\NJOY2012\77C_0001PCT\u236\u236_0001PCT.bat
C:\NJOY2012\77C_0001PCT\u238\u238_0001PCT.bat
C:\NJOY2012\78C_20PCT\u234\u234_20PCT.bat
C:\NJOY2012\78C_20PCT\u235\u235_20PCT.bat
C:\NJOY2012\78C_20PCT\u236\u236_20PCT.bat
C:\NJOY2012\78C_20PCT\u238\u238_20PCT.bat
C:\NJOY2012\79C_30PCT\u234\u234_30PCT.bat
C:\NJOY2012\79C_30PCT\u235\u235_30PCT.bat
C:\NJOY2012\79C_30PCT\u236\u236_30PCT.bat
C:\NJOY2012\79C_30PCT\u238\u238_30PCT.bat
echo Test complete, regard all further alarms!
```

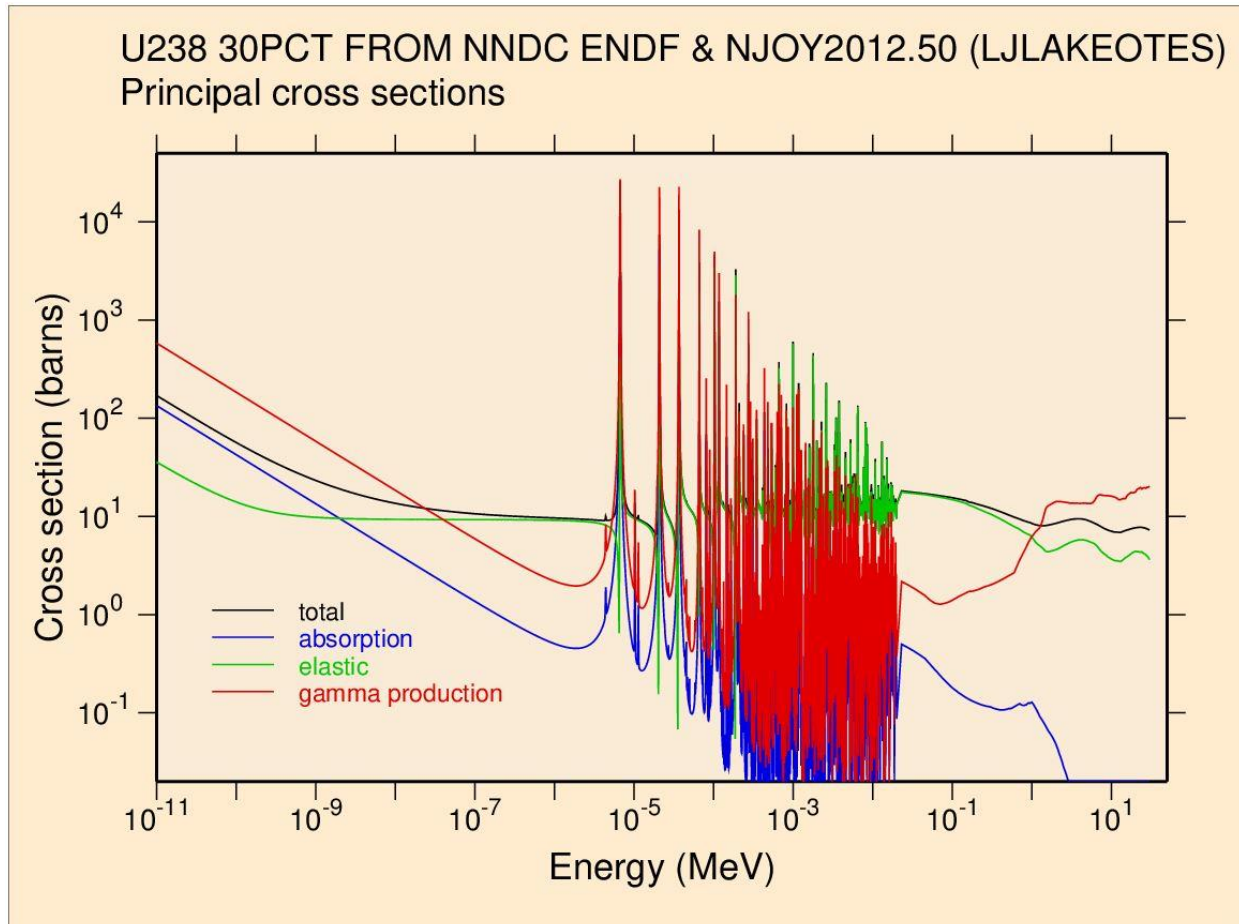
APPENDIX H: NJOY2012 CROSS-SECTION PLOTS

Copy of NJOY Cross-section Plots for U-234 and 30PCT









APPENDIX I: XSDIR FILE

XSDIR File entries from NJOY for MCNP6\X usage

01/10/2016

directory

92234.70c	232.030400	92234.70c	0	1	1	446012	0	0	2.585E-08	ptable
92235.70c	233.024800	92235.70c	0	1	1	812025	0	0	2.585E-08	ptable
92236.70c	234.017800	92236.70c	0	1	1	370091	0	0	2.585E-08	ptable
92238.70c	236.005800	92238.70c	0	1	1	1597077	0	0	2.585E-08	ptable
92234.71c	232.030400	92234.71c	0	1	1	447281	0	0	2.585E-08	ptable
92235.71c	233.024800	92235.71c	0	1	1	813516	0	0	2.585E-08	ptable
92236.71c	234.017800	92236.71c	0	1	1	371395	0	0	2.585E-08	ptable
92238.71c	236.005800	92238.71c	0	1	1	1598446	0	0	2.585E-08	ptable
92234.72c	232.030400	92234.72c	0	1	1	447281	0	0	2.585E-08	ptable
92235.72c	233.024800	92235.72c	0	1	1	813489	0	0	2.585E-08	ptable
92236.72c	234.017800	92236.72c	0	1	1	371395	0	0	2.585E-08	ptable
92238.72c	236.005800	92238.72c	0	1	1	1598437	0	0	2.585E-08	ptable
92234.73c	232.030400	92234.73c	0	1	1	447281	0	0	2.585E-08	ptable
92235.73c	233.024800	92235.73c	0	1	1	813569	0	0	2.585E-08	ptable
92236.73c	234.017800	92236.73c	0	1	1	371395	0	0	2.585E-08	ptable
92238.73c	236.005800	92238.73c	0	1	1	1598437	0	0	2.585E-08	ptable
92234.74c	232.030400	92234.74c	0	1	1	447338	0	0	2.585E-08	ptable
92235.74c	233.024800	92235.74c	0	1	1	813489	0	0	2.585E-08	ptable
92236.74c	234.017800	92236.74c	0	1	1	371395	0	0	2.585E-08	ptable
92238.74c	236.005800	92238.74c	0	1	1	1598437	0	0	2.585E-08	ptable
92234.75c	232.030400	92234.75c	0	1	1	447281	0	0	2.585E-08	ptable
92235.75c	233.024800	92235.75c	0	1	1	813569	0	0	2.585E-08	ptable
92236.75c	234.017800	92236.75c	0	1	1	371395	0	0	2.585E-08	ptable
92238.75c	236.005800	92238.75c	0	1	1	1598437	0	0	2.585E-08	ptable
92234.76c	232.030400	92234.76c	0	1	1	447281	0	0	2.585E-08	ptable
92235.76c	233.024800	92235.76c	0	1	1	813569	0	0	2.585E-08	ptable
92236.76c	234.017800	92236.76c	0	1	1	371395	0	0	2.585E-08	ptable
92238.76c	236.005800	92238.76c	0	1	1	1598437	0	0	2.585E-08	ptable
92234.77c	232.030400	92234.77c	0	1	1	447281	0	0	2.585E-08	ptable
92235.77c	233.024800	92235.77c	0	1	1	813516	0	0	2.585E-08	ptable
92236.77c	234.017800	92236.77c	0	1	1	371395	0	0	2.585E-08	ptable
92238.77c	236.005800	92238.77c	0	1	1	1598437	0	0	2.585E-08	ptable
92234.78c	232.030400	92234.78c	0	1	1	447281	0	0	2.585E-08	ptable
92235.78c	233.024800	92235.78c	0	1	1	813525	0	0	2.585E-08	ptable
92236.78c	234.017800	92236.78c	0	1	1	371386	0	0	2.585E-08	ptable
92238.78c	236.005800	92238.78c	0	1	1	1598446	0	0	2.585E-08	ptable
92234.79c	232.030400	92234.79c	0	1	1	447281	0	0	2.585E-08	ptable
92235.79c	233.024800	92235.79c	0	1	1	813525	0	0	2.585E-08	ptable
92236.79c	234.017800	92236.79c	0	1	1	371386	0	0	2.585E-08	ptable
92238.79c	236.005800	92238.79c	0	1	1	1598455	0	0	2.585E-08	ptable
92234.50c	232.030000	endf5p	0	1	222941	89433	0	0	2.53E-08	
92235.50c	233.025000	rmccs	0	1	395843	60489	0	0	2.53E-08	
92236.50c	234.018000	endf5p	0	1	245312	138715	0	0	2.53E-08	
92238.50c	236.006000	rmccs	0	1	415408	88998	0	0	2.53E-08	
92234.86c	232.0304	92234.716nc	0	1	4	427480	0	0	2.1543E-08	ptable
92235.86c	233.0248	92235.716nc	0	1	4	876775	0	0	2.1543E-08	ptable
92236.86c	234.0178	92236.716nc	0	1	4	358841	0	0	2.1543E-08	ptable
92238.86c	236.0058	92238.716nc	0	1	4	1690077	0	0	2.1543E-08	ptable
1001.50c	0.999170	rmccs	0	1	1	2766	0	0	2.53E-08	
6000.50c	11.896900	rmccs	0	1	17298	23326	0	0	2.53E-08	
7014.50c	13.883000	rmccs	0	1	28986	45457	0	0	2.53E-08	
8016.50c	15.858000	rmccs	0	1	40363	37942	0	0	2.53E-08	
13027.50c	26.750000	rmccs	0	1	84704	54162	0	0	2.53E-08	
lwtr.01t	0.000000	tmccs	0	1	1	10193	0	0	2.58519E-08	

APPENDIX J: MCNP6/X INPUT FILES

Copy of the MCNP6\X input decks for HMF-001

Idealized HEU Shell Exp from LA4208. Six Shells. 05/12/93.

```
1  1 4.8150E-02 -1      imp:n=1
2  7 5.0306E-05  1  -2 imp:n=1
3  2 4.8154E-02  2  -3 imp:n=1
4  7 5.0306E-05  3  -4 imp:n=1
5  3 4.8154E-02  4  -5 imp:n=1
6  7 5.0306E-05  5  -6 imp:n=1
7  4 4.8152E-02  6  -7 imp:n=1
8  7 5.0306E-05  7  -8 imp:n=1
9  5 4.8154E-02  8  -9 imp:n=1
10 6 4.7780E-02  9 -10 imp:n=1
11 0                      10 imp:n=0
```

```
1  so 1.0216
2  so 1.0541
3  so 6.2809
4  so 6.2937
5  so 7.7525
6  so 7.7620
7  so 8.2527
8  so 8.2610
9  so 8.7062
10 so 8.7499
```

```
m1 92235.50c 4.4936E-02 92238.50c 2.7213E-03 92234.50c 4.9357E-04
m2 92235.50c 4.5244E-02 92238.50c 2.4168E-03 92234.50c 4.9357E-04
m3 92235.50c 4.5268E-02 92238.50c 2.3930E-03 92234.50c 4.9357E-04
m4 92235.50c 4.5090E-02 92238.50c 2.5690E-03 92234.50c 4.9357E-04
m5 92235.50c 4.5239E-02 92238.50c 2.4215E-03 92234.50c 4.9357E-04
m6 92235.50c 4.4874E-02 92238.50c 2.4169E-03 92234.50c 4.8974E-04
m7 7014.50c 3.5214E-05 8016.50c 1.5092E-05
kcode 3000 1.0 10 1500
ksrc 0. 0. 0.
f1:n 10
sd1 10
e1 1-12 1-11 1-10 1-9 1-8 1-7 1-6 1-5 1-4 1-3 1-2 .1 1 18i 20
print
```

Copy of the MCNP6\X input decks for HMF-004

```

Idealized HEU sphere (97.675 w/o) in sphere of H2O TANS 27, 412 (11/77)
1 1 0.048143 -1 $ HEU sphere
2 2 0.10021 1 -2 $ water sphere
3 0 2 $ infinity

1. so 6.5537 $ radius of HEU sphere
2 so 33.471 $ radius of water sphere

mode n
kcode 5000 1.0 20 220
imp:n 1.0 1.0 0.0
sdef cel=1 erg=d1 rad=d2 pos=0.0 0.0 0.0
sp1 -3
si2 0.0 0.65537
sp2 -21 2
vol 1179.1 155891. 0.0
area 539.74 14078.
c HEU (97.675 w/o)
m1 92234.50c 0.011150
92235.50c 0.97694
92236.50c 0.0019919
92238.50c 0.0099250
c Water
m2 1001.50c 0.66667
8016.50c 0.33333
mt2 lwtr.01t
totnu
prdmp j 110
fl:n 1
sd1 1
e1 1-12 1-11 1-10 1-9 1-8 1-7 1-6 1-5 1-4 1-3 1-2 .1 1 18i 20
print

```

APPENDIX K: MCNP6\X DOS BATCH FILES

MCNP6 DOS Batch File

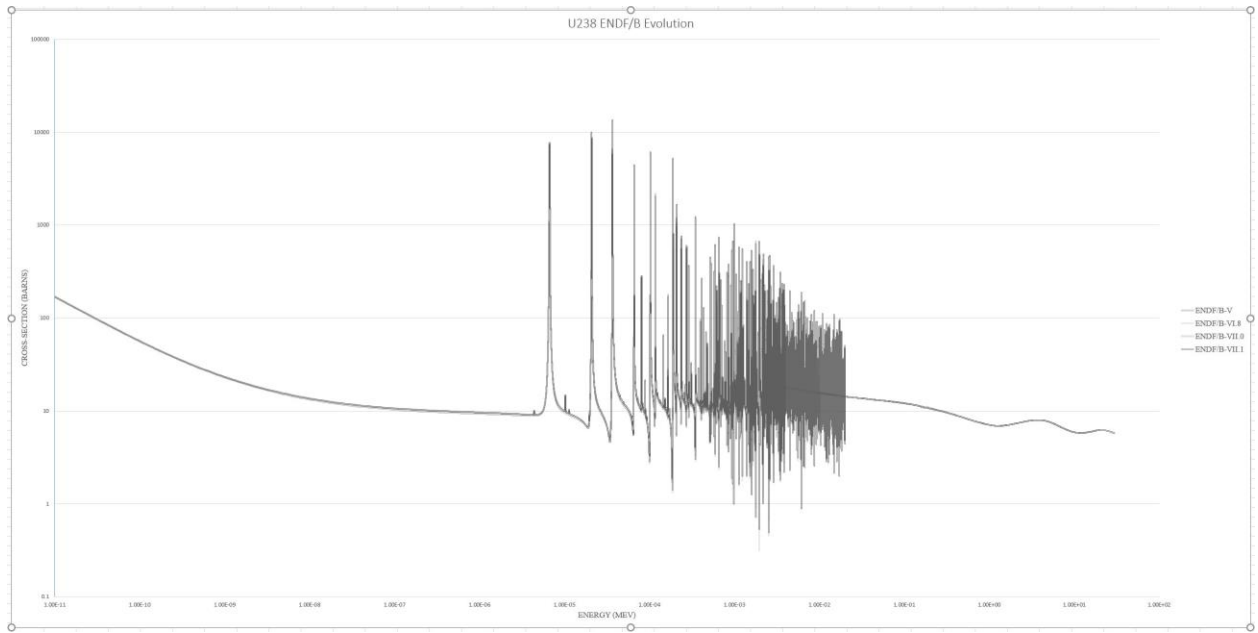
```
echo Base-70c
mcnp6.exe i=hmf_001_base.txt o=hmf_001_base_out.txt
mcnp6.exe i=hmf_004_base.txt o=hmf_004_base_out.txt
echo 10PCT-71c
mcnp6.exe i=hmf_001_10PCT.txt o=hmf_001_10PCT_out.txt
mcnp6.exe i=hmf_004_10PCT.txt o=hmf_004_10PCT_out.txt
echo 05pct-72c
mcnp6.exe i=hmf_001_05PCT.txt o=hmf_001_05PCT_out.txt
mcnp6.exe i=hmf_004_05PCT.txt o=hmf_004_05PCT_out.txt
echo 01pct-73c
mcnp6.exe i=hmf_001_01PCT.txt o=hmf_001_01PCT_out.txt
mcnp6.exe i=hmf_004_01PCT.txt o=hmf_004_01PCT_out.txt
echo 005pct-74c
mcnp6.exe i=hmf_001_005PCT.txt o=hmf_001_005PCT_out.txt
mcnp6.exe i=hmf_004_005PCT.txt o=hmf_004_005PCT_out.txt
echo 001pct-75c
mcnp6.exe i=hmf_001_001PCT.txt o=hmf_001_001PCT_out.txt
mcnp6.exe i=hmf_004_001PCT.txt o=hmf_004_001PCT_out.txt
echo 0005pct-76c
mcnp6.exe i=hmf_001_0005PCT.txt o=hmf_001_0005PCT_out.txt
mcnp6.exe i=hmf_004_0005PCT.txt o=hmf_004_0005PCT_out.txt
echo 0001pct-77c
mcnp6.exe i=hmf_001_0001PCT.txt o=hmf_001_0001PCT_out.txt
mcnp6.exe i=hmf_004_0001PCT.txt o=hmf_004_0001PCT_out.txt
echo 20PCT-78c
mcnp6.exe i=hmf_001_20PCT.txt o=hmf_001_20PCT_out.txt
mcnp6.exe i=hmf_004_20PCT.txt o=hmf_004_20PCT_out.txt
echo 30PCT-79c
mcnp6.exe i=hmf_001_30PCT.txt o=hmf_001_30PCT_out.txt
mcnp6.exe i=hmf_004_30PCT.txt o=hmf_004_30PCT_out.txt
echo Base-50c
mcnp6.exe i=hmf_001_50.txt o=hmf_001_50_out.txt
mcnp6.exe i=hmf_004_50.txt o=hmf_004_50_out.txt
echo Base-86c
mcnp6.exe i=hmf_001_86.txt o=hmf_001_86_out.txt
mcnp6.exe i=hmf_004_86.txt o=hmf_004_86_out.txt
```

MCNPX DOS Batch File

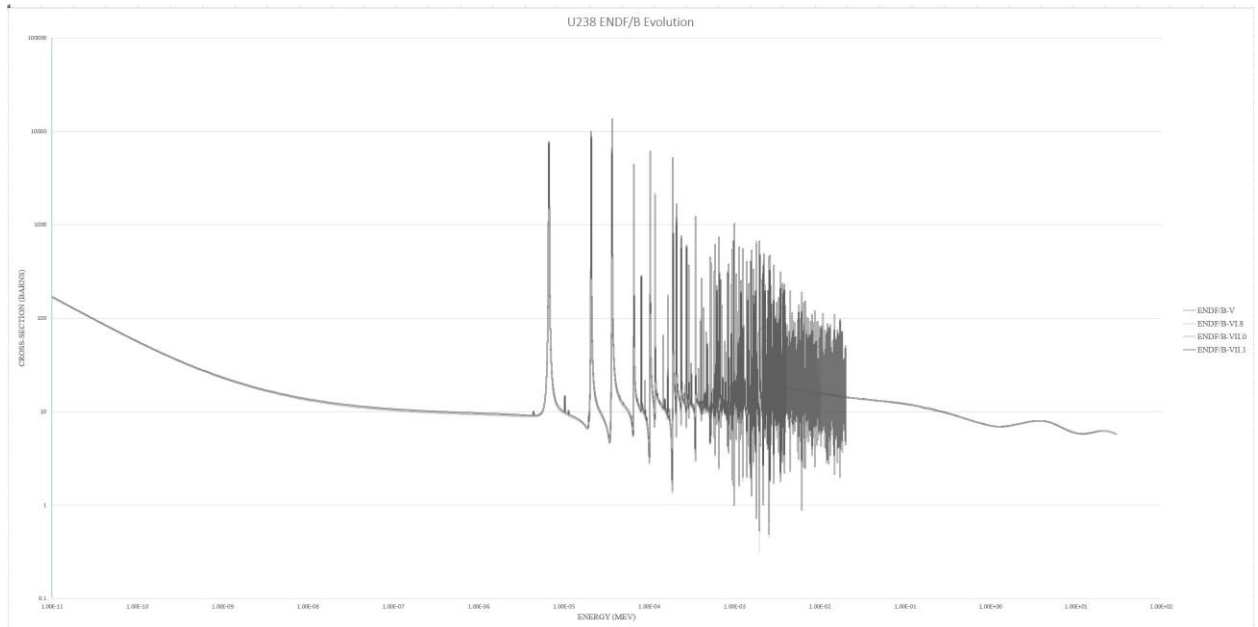
```
echo Base-70c
mcnpx.exe i=hmf_001_base.txt o=hmf_001_base_out.txt
mcnpx.exe i=hmf_004_base.txt o=hmf_004_base_out.txt
echo 10PCT-71c
mcnpx.exe i=hmf_001_10PCT.txt o=hmf_001_10PCT_out.txt
mcnpx.exe i=hmf_004_10PCT.txt o=hmf_004_10PCT_out.txt
echo 05pct-72c
mcnpx.exe i=hmf_001_05PCT.txt o=hmf_001_05PCT_out.txt
mcnpx.exe i=hmf_004_05PCT.txt o=hmf_004_05PCT_out.txt
echo 01pct-73c
mcnpx.exe i=hmf_001_01PCT.txt o=hmf_001_01PCT_out.txt
mcnpx.exe i=hmf_004_01PCT.txt o=hmf_004_01PCT_out.txt
echo 005pct-74c
mcnpx.exe i=hmf_001_005PCT.txt o=hmf_001_005PCT_out.txt
mcnpx.exe i=hmf_004_005PCT.txt o=hmf_004_005PCT_out.txt
echo 001pct-75c
mcnpx.exe i=hmf_001_001PCT.txt o=hmf_001_001PCT_out.txt
mcnpx.exe i=hmf_004_001PCT.txt o=hmf_004_001PCT_out.txt
echo 0005pct-76c
mcnpx.exe i=hmf_001_0005PCT.txt o=hmf_001_0005PCT_out.txt
mcnpx.exe i=hmf_004_0005PCT.txt o=hmf_004_0005PCT_out.txt
echo 0001pct-77c
mcnpx.exe i=hmf_001_0001PCT.txt o=hmf_001_0001PCT_out.txt
mcnpx.exe i=hmf_004_0001PCT.txt o=hmf_004_0001PCT_out.txt
echo 20PCT-78c
mcnpx.exe i=hmf_001_20PCT.txt o=hmf_001_20PCT_out.txt
mcnpx.exe i=hmf_004_20PCT.txt o=hmf_004_20PCT_out.txt
echo 30PCT-79c
mcnpx.exe i=hmf_001_30PCT.txt o=hmf_001_30PCT_out.txt
mcnpx.exe i=hmf_004_30PCT.txt o=hmf_004_30PCT_out.txt
echo Base-50c
mcnpx.exe i=hmf_001_50.txt o=hmf_001_50_out.txt
mcnpx.exe i=hmf_004_50.txt o=hmf_004_50_out.txt
echo Base-86c
mcnpx.exe i=hmf_001_86.txt o=hmf_001_86_out.txt
mcnpx.exe i=hmf_004_86.txt o=hmf_004_86_out.txt
```

APPENDIX L: ENDF/B EVOLUTION

U-235



U-238



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Thesis Title

Neutron Cross-Section Sensitivity Studies in Higher Actinides for Criticality Safety in Reprocessing

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