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NEUTRON CROSS-SECTION SENSITIVITY STUDIES IN HIGHER ACTINIDES

FOR CRITICALITY SAFETY IN REPROCESSING

by

Lawrence J. Lakeotes

Bachelor of Science Auburn University, Auburn 1997

A thesis submitted in partial fulfillment of the requirements for the

Master of Science Degree in Mechanical Engineering Department of Mechanical Engineering Howard R. Hughes College of Engineering

> Graduate Coliege University of Nevada, Las Vegas May 2008

UMI Number: 1456349

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April 04_{.20}08

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Entitled

Neutron Cross-Section Sensitivity Studies in Higher Actinides for

Criticality Safety in Reprocessing

is approved in partial fulfillment of the requirements for the degree of

Master of Science in Mechanical Engineering

Examination Committee Chair

Dean of the Graduate College

Examination Committee Member

Examination Committee Member

Examination Committee Member

Graduate College Faculty Representative

ABSTRACT

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

by

Lawrence J. Lakeotes

Dr. Robert Boehm, Examination Committee Chair Professor of Mechanical Engineering University of Nevada, Las Vegas

During reprocessing, the spent fuel rod can be divided up into its component parts for separation into different waste streams. These radioactive streams are then directed appropriately toward low-level waste (LLW) storage, high-level waste (HLW) storage, or reuse into a recycled fuel pin. [1]

The issue that requires evaluation is the nuclear reaction of the higher actinides in reprocessing in an aqueous solution with regard to small temperature changes. This will need an analysis of neutron cross section, which is the measure of the probability that a nuclear reaction will occur.

The isotopes' cross sections need to be temperature corrected. This will have a direct effect on the reactivity per gram for an isotope being reprocessed. [2] These specific cross sections were computed using NJOY version 99.259 with ENDF/B-VII data and applying it toward the criticality code MCNP5.

The process entailed research into the structure of the ENDF file format, established criticality benchmarks, and formulated hard spectrum cross sections from the ENDF data with NJOY. It also required analyzing the reactivity changes to each actinide, (Np-237, Pu-239, Pu-240, Pu-241, Am-241, Am-242m, Am-243, and Cm-244), as well as formulating soft spectrum cross sections. The contribution of each actinide on the total reactivity difference of the solution needs to be carefully calculated with regard to small changes in density and temperature. [2]

The study showed that the small change in temperature from 273.15 K to 313.15 K did not have an impact on the reactivity per gram. This was analyzed for all eight of the isotopes in the fast spectrum.

This methodology will establish a process for UNLV to commence work into cross-section analysis and reactivity sensitivity studies. It will also produce the research into the formulation of the fast and thermal cross sections for the higher actinides and the calculations for changes in reactivity of the hard spectrum with small changes in temperature.

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LIST OF ABBREVIATIONS

ACER	NJOY MODULE TO PRODUCE NCMP DATA LIBRARY
AENCF/AFGE	AVERAGE ENERGY OF NEUTRONS CAUSING FISSION
Am	AMERICIUM
ANL	ARGONNE NATIONAL LABORATORY
BROADR	NJOY MODULE TO ADD TEMPERATURE DEPENDANCE
	TO POINTWISE CROSS SECTIONS
CI	
Cm	CURIUM
cm	CENTIMETER
DOE	DEPARTMENT OF ENERGY
FALE	ENERGY OF AVERAGE LETHARGY CAUSING FISSION
ENDE	EVALUATED NUCLEAR DATA FILES
ENDE/B	EVALUATED NUCLEAR DATA FILES/B FORMAT
a	GRAM
GASPR	NIOY MODULE FOR PRODUCING GAS PRODUCTION DATA
GENDE	GROUPWISE EVALUATED NUCLEAR DATA FILES
HEATR	NIOY MODULE FOR CALCULATING KERMA AND DAMAGE
HIW	HIGH LEVEL WASTE
HELL	
IFU	
IHECSBE	INTERNATIONAL HANDBOOK OF EVALUATED CRITICALITY
INCODE	SAFETY BENCHMARK EXPERIMENTS
INI	
K	
KCODE	MCNP MODULE FOR CALCULATING CRITICALITY
kere	FEECTIVE NEUTRON MULTIPLICATION FACTOR
KERMA	
IANI	LOS ALAMOS NATIONAL LABORATORY
IBTI	LOWER BOUND THRESHOLD LIMIT
LEU	
	LOW LEVEL WASTE
MCNP	MONTE CARLO N-PARTICI E TRANSPORT CODE
MFT	METAI
MeV	MEGA ELECTRON VOI T
MODER	NJOY MODULE FOR ASCILTO/FROM BINARY CONVERSION
MF	ENDF MATERIAL FILE

MT	ENDF MATERIAL SECTION
MTHM	METRIC TON HEAVY METAL
NJOY	NUCLEAR DATA PROCESSING SYSTEM SOFTWARE
NNDC	NATIONAL NUCLEAR DATA CENTER
Np	NEPTUNIUM
ORNL	OAK RIDGE NATIONAL LABORATORY
PENDF	POINTWISE EVALUATED NUCLEAR DATA FILES
Pu	PLUTONIUM
PURR	NJOY MODULE FOR UNRESOLVED PROBABILITY TABLES
r	RADIUS
ROA	RANGE OF APPLICABILITY
ROP	RANGE OF PARAMETERS
RSICC	RADIATION SAFETY INFORMATION COMPUTATIONAL
	CENTER
SMF	SPECIAL METAL FAST
SNF	SPENT NUCLEAR FUEL
SNL	SANDIA NATIONAL LABORTORY
THERMR	NJOY MODULE FOR COMPUTING SCATTERING EFFECTS
U	URANIUM
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
XSDIR	MCNP CROSS SECTION DIRECTORY FILE
YMP	YUCCA MOUNTAIN PROJECT

ACKNOWLEDGMENTS

The author would like to express his thanks to Dr. Denis Beller (UNLV), Dr. Charlotta Sanders (YMP/UNLV), Dr. Robert Boehm (UNLV), Dr. Kenneth Czerwinski (UNLV), Dr. Larry Sanchez (SNL), Dr. Skip Kahler (LANL), Dr. Michael Dunn (ORNL), Dr. Robert Busch (UNM), Dr. Candido Pereira, (ANL), Dr. Mohamad Trabia, (UNLV), Timothy Beller (UNLV), and Ryan LeCounte (UNLV) for their help with providing information, software knowledge, and editorial work in the production of this document. Thanks are also expressed to the Department of Energy for the grant to conduct the research, to the technical staff of the Radiation Safety Information Computational Center (RSICC) for maintaining access to the required software, and to National Securities Technology, LLC for providing time to conduct the research. I would of course like to thank my wife Te Ann Marie Lakeotes for her patience, understanding, and love.

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CHAPTER 1

INTRODUCTION

The Yucca Mountain Project's (YMP) ability to hold radioactive High Level Waste (HLW) is constrained by space and heat loading from the decay of fission products in the spent nuclear fuel (SNF). It has been roughly calculated that the site can hold about 125,000 metric tons of heavy metal (MTHM). Statutorily, the YMP is currently limited to 77,000 MTHM. To date of this paper, there is about 60,000 MTHM from commercial and military reactors, and that volume is growing at the nuclear power plants' dry storage areas. This amount of HLW contains all of the used and unspent fuel. The unspent fuel is about 90% of the fuel assembly, which is a function of the burn-up rate. [3]

If the unspent fuel could be extracted and reprocessed, it would alleviate future energy requirements. It would also reduce the total amount of waste to be stored at the geological repository in Yucca Mountain. This would extend the storage capabilities of the proposed repository so that a new disposal site would not be needed for well into the 22nd century.

Because limited space is available for the Yucca Mountain repository, reprocessing of spent fuel is becoming a viable resource for closing the nuclear fuel cycle. This will enable the recovery of unspent fuel. [4] If reprocessing is

going to become a reality, then the first requirement will be to establish criticality safety limits for the potential reprocessing facility in the United States.

Reprocessing can be conducted in several forms. The uranium extraction process (UREX+1) is the current method of choice at Argonne National Laboratory (ANL). [5] The UREX +1 process is a series of four solvent-extraction processes and one ion exchange process that perform the following operations: (1) recovery of Uranium (U) and Technecium (Tc), (2) recovery of Cesium (Cs) and Strontium (Sr), (3) recovery of Plutonium (Pu), Neptunium (Np), minor actinides and lanthanides Americium (Am) and Curium (Cm), (4) and separation of actinides from lanthanides. [5]

This will allow a trifecta of efficiencies for the YMP. It will first produce a large reduction in heat load for the geological repository from the long-lived actinides; it will allow the reuse of unspent fuel and bred plutonium; and it will also reduce the amount of material heading for geological storage, thus increasing the usage of Yucca Mountain and delaying the requirement for a second repository.

Purpose of the Study

A criticality safety study has not currently been conducted using fast or thermal cross sections from the higher actinides, to determine reactivity changes for the temperatures of reprocessing. Unfortunately, limited data are available for the higher actinides, so calculations and experiments are required to be conducted to determine the thermal cross sections. Once the thermal cross

sections are confirmed, then historic benchmarks will need to be compared in order to establish a preliminary upper subcritical limit (USL).

The Brookhaven National Laboratory (BNL) maintains the database for the evaluated nuclear data files (ENDF). ENDF data is the parameterization and reduction of analyzed experimentally measured cross-section data coupled with the predictions of nuclear model calculations. This attempts to produce the true value of a cross section. The current data from BNL is ENDF/B-VII, and this input will be used for refining the ENDF cross sections to the usable cross sections for temperatures that approximate reprocessing.[6]

Idaho National Laboratory (INL) maintains the library of criticality benchmark experiments. The data retained in this library describe the prior benchmarks and provide parameters for the establishment of the upper subcritical limits. Experiments with the higher actinides are limited in number, so that computational methods of extrapolation are required to find possible solutions for current higher actinide reactivity changes.

No previous work has been found to be documented in this area. Conducting research into this field will advance the ability to commence reprocessing sooner in the United States, rather than later.

Research Questions

How does reactivity change with a rise or fall in temperature for reprocessing? The main focus of this research is to determine the upper limit for k_{eff} when reprocessing, due to the temperature changes.

The criticality benchmark experiments will be reviewed for applicable parameter, for inclusion into the study. Once the benchmarks with similar characteristics are selected, then the range of applicability for the future benchmark will be chosen. Once the parameters are selected, then the USL can be calculated.

The latest Evaluated Nuclear Data Files (ENDF/B-VI and VII) from Brookhaven National Laboratory will be used to obtain the basic actinide properties for Np-237, Pu-239, Pu-240, Pu-241, Am-241, Am-242m, Am-243, and Cm-244. These isotopes are selected for this research due to being the key isotopes involved in the reprocessing efforts. The available ENDF data will be used by the software NJOY version 99.259 to temperature-correct, and reconstruct the point-wise cross-sections from the ENDF data files. [7]

The MCNP version 5.1 software will then be used to evaluate the crosssection of the material in the Dirty Jezebel (20.4% Pu-240) and Flattop structures for the initial computational criticality studies. [8] The Dirty Jezebel experiments were conducted at Los Alamos National Laboratory (LANL) in the 1960s to conduct reactivity worth measurements. It was a simple four-part sphere with a void for replacement measurements. The Flattop experiments were conducted at LANL in the mid-1990s. Flattop was a sphere inside of a sphere model with a glory hole to conduct replacement measurements. A glory hole is a void inside the inner sphere where a sample isotope is placed and the resulting change in reactivity is measured by the increase or decrease in neutron flux.[9]

The temperature of the higher actinides in the models will be changed in small increments to determine reactivity changes for the fixed volume and concentration of that stream. This difference in reactivity between the void and replacement criticality runs will then be divided by the mass (in grams) of the replacement sample. This will produce the reactivity per gram from the higher actinide isotopes. The output of these calculations will then be used to evaluate the process for accuracy.

Significance of the Study

A criticality safety study must be done to ensure that the amount of fissile material in the aqueous solution stays below the required amount of material to prevent a critical mass from forming. DOE nuclear facilities are to be designed and constructed in a manner that ensures adequate protection to the public, workers, and the environment from nuclear hazards. [10]

The safety level is determined by defining and limiting k_{eff} in a system or process. The k_{eff} is the number of neutrons born from all sources in the system in the current generation divided by the number of neutrons born in the previous generation from all sources. [11] The neutron population includes prompt, delayed, and source neutrons.

In order to reprocess, a k_{eff} of less than one (usually less than 0.95) will be required for personnel protection and safe reprocessing. [10] The k_{eff} is calculated by using the fissile material mass, density, cross sections, moderator material, reflector material, and the geometry into consideration for determining

resulting k_{eff} and reactivity changes. If reprocessing can not be safely conducted, then a criticality accident can occur, just like in the fuel precipitation plant at Tokai-mura, Japan on 30 Sept 1999. [12]

CHAPTER 2

REVIEW OF RELATED LITERATURE

Previous Research

Nuclear research is an ongoing process to improve the quality of data available for the scientific community. [13] Some of the ongoing issues involve missing sections of experimental data in the National Nuclear Data Center (NNDC) collection. Reprocessing has been discussed at length, but criticality safety studies have not been mentioned. [1]

Conducting a criticality safety study necessitates that the latest in nuclear data from NNDC. This will require that NNDC's ENDF/B-VII data be verified by currently established benchmark models prior to conducting any new research. [14] Current efforts are ongoing to establish correlations between the benchmarks from ENDF/B-VI, JEF 3.1 and the new ENDF/B-VII data sets. [15] This will forward the progress of creating new cross sections for generating benchmarks with improved accuracy. [16]

Criticality Benchmark Experiments

In order to properly prepare for the criticality calculations required for reprocessing, an in depth study of previous benchmarks is necessary. This

approach allows a step-by-step analysis of pertinent parameters, as spelled out by U.S. Department of Energy (DOE) requirements. [10]

An exhaustive search through all the criticality benchmark experiments from the 2007 International Handbook of Evaluated Criticality Safety Benchmark Experiments (IHECSBE) provided many benchmarks to choose from, but only a few that would parallel the desired intent to directly provide an experiment for obtaining cross-sections from the higher actinides that are in this research. [9] The end result of this research will be to analyze fast cross sections of the higher actinides.

There are several AGN-201 reactors located across the United States, (University of New Mexico, Texas A&M, and Oregon State University are a few examples). The AGN-201 reactor is a compact, self-contained, graphitemoderated research and training reactor that is licensed to operate at a maximum thermal power of 5 Watts. It utilizes four fueled control elements which are inserted from the bottom of the core. The control elements contain fuel disks which consist of nominally 20% enriched uranium dioxide dispersed in polyethylene medium. [17]

The 2007 IHCSBE is divided into eight sections. The ones that will be referenced here are Volume I (Plutonium Systems), Volume II (Highly Enriched Uranium Systems), Volume III (Intermediate and Mixed Uranium Systems), Volume IV (Low Enriched Uranium), Volume V (Uranium-233 Systems), and Volume VII (Special Isotope Systems). Each volume contains specific

benchmarks divided into four categories: metal systems, compound systems, solutions systems, and miscellaneous systems. [9]

The benchmarks are based on historic experiments that were conducted from the 1940s to the present. Each of the benchmarks is documented in such a way so that it can be reproduced. Each individual benchmark includes a detailed description of the benchmark, an evaluation of the experimental data, the benchmark's specifications, the result of the sample calculations, and pertinent references. [15]

The benchmark experiments that were selected from Volume I were PU-MET-FAST-001 (20.1% Pu-240 Jezebel), PU-MET-FAST-002 (20.1% Pu-240 Jezebel), and PU-MET-FAST-006 (Flattop). These three were selected due to their plutonium composition and comparisons with Pu-239, Pu-240, and Pu-241 and were reviewed due to their fast neutron spectrums and simple geometric construction.

Three benchmarks from Volume II are referenced, HEU-MET-FAST-001 (Godiva), HEU-MET-FAST-008, and HEU-MET-FAST-018 (Planet). These are useful for the enriched uranium spectrum, but they do not have the range of parameters required to fit this research.

Volume III contains the Intermediate and Mixed Uranium Systems. The benchmarks in this volume start at 10% 235-U enrichment and expand up to 93%. The volume also contains benchmarks that have mixtures of thorium, plutonium and depleted uranium. IEU-MET-FAST-001 (Jemima), IEU-MET-FAST-003, IEU-MET-FAST-004, IEU-MET-FAST-009, and the IEU-COMP-

THERM-003 (TRIGA) benchmarks were reviewed due to the lower fissile material composition.

Volume IV contains the Low Enriched Uranium benchmarks. The enrichments are from 1.6% to 10% uranium enrichment. LEU-COMP-THERM-002 was selected for comparison of thermal data with the other fast benchmarks.

Only one benchmark from Volume V, Uranium-233 Systems, was selected. This was conducted to have a comparison of a different isotope and enrichment. This is due to all the other experiments on this volume have geometries that do not fit our range of parameters for a simple sphere.

The last volume is Volume VII for Special Isotope Systems. Three benchmarks were selected from this volume: SPEC-MET-FAST-001 (20.1% Pu-240 Jezebel), SPEC-MET-FAST-002 (20.1% Pu-240 Jezebel), and SPEC-MET-FAST-003 (Flattop HEU). These three were selected for the replacement data that were available for Np-237, Pu-239, and Cm-244. They were also selected for their fast spectrums and simple geometries.

Criticality Limit Establishment

The proposed analysis methods and neutron cross-section data will be benchmarked by comparison with critical experiments from the IHECSBE. This will qualify the applications and the computer environment. The critical experiments used for benchmarking will include, to the extent possible, configurations having neutronic and geometric characteristics similar to those of the proposed system. [18]

Table '	1.	Range	of Ap	plicability
---------	----	-------	-------	-------------

Category/ Description	Parameter		
	Fissionable Element		
Meterials (Fiscis solution	Physical Form		
Materials/ Fissionable Material	Isotopic Composition		
matorial	Atomic Density (atoms/b-cm)		
	Temperature		
	Element		
	Physical Form		
Materials/ Moderator	Atomic Density (atoms/b-cm)		
	Ratio to fissile material		
	Temperature		
Materials/ Reflector	Material/ Physical Form		
	Element		
Materials/ Neutron Absorber	Physical Form		
	Atomic Density (atoms/b-cm)		
Goometry	Heterogeneity		
Geometry	Shape		
	AENCF (MeV)		
	EALF (MeV)		
	Neutron Flux Energy Spectra Thermal (T) =		
	Intermediate(I) =		
	Fast(F) =		
Neutron Energy	Fission Rate vs Neutron Energy Thermal (T) =		
	Intermediate(I) =		
	Fast(F) =		
	Capture Rate vs Neutron Energy Thermal (T) =		
	Intermediate(I) =		
	Fast(F) =		

The range of parameters (ROP) includes the desired characteristics from the reprocessing system to be applied to the benchmarks. The range of applicability (ROA) is the characteristics of the benchmarks that can be applied to the

reprocessing system. When the ROA and the ROP are matched as close as possible, then the next step will be to determine the Upper Subcritical Limit(USL).

Establishing an USL requires: (1) selection of benchmark experiments; (2) determination of the range of applicability of the benchmark experiments; (3) establishment of a lower-bound tolerance limit; and, if necessary, (4) setting the penalties for extending the range of applicability.

The first step in conducting a criticality study is to review the previous historical benchmarks. Once the appropriate benchmarks are selected, then the process of establishing the new USL begins.

The range of applicability has six groups for data review: Materials/ Fissionable Material, Materials/ Moderator, Materials/ Reflector, Materials/ Neutron Absorber, Geometry, and Neutron Energy.

The Fissionable Material is categorized by the fissionable element, physical form, isotopic composition, and temperature. The physical form and fissionable element are the priority parameters. The element needs to be the same or the spectra will not be comparable. The physical form needs to be similar, but not exact, in order to have comparable leakage factors.

The second, third and fourth areas of the range of applicability are the Moderator, Reflector, and Neutron Absorber sections. Since none of the fast benchmarks under review have moderators, reflectors, or neutron absorbers, these characteristics are not required for the analysis.

The Geometry section is for comparison of the type of heterogeneous or homogeneous mixture types and for the basic shape of the experimental models.

This ensures that lattice array models are not used for simple sphere experiments.

The neutron energy section presents the average energy of neutrons causing fission (AENCF/AFGE) and average neutron lethargy causing fission (EALF) for review. This information will indicate what neutron spectrum is present for the experimental model. Trend analysis by graphing all of the AENCFs for the reviewed benchmarks will indicate what energy band the benchmark should fall in, provided it has similar parameters.

Now that the ROP and ROA have been matched as closely as possible, and all outlying parameters are understood and accepted, it is time to proceed with calculating the USL. Determining the Lower Bound Tolerance Limit (LBTL) is the first step in calculating the Upper Subcritical Limit (USL).

This is done by plotting the AENCF versus k_{eff} for the similarly selected criticality benchmarks. Observe the AENCF energy levels and use the following equations to determine the LBTL. If the AENCFs from the benchmarks are:

0 MeV < AENCF < 0.1679 MeV,

then the LBTL=0.96797.

If the AENCFs are between:

0.1679 MeV < AENCF < 0.902 MeV,

then the LBTL = (-1.366e-2*AENCF) + 0.970271.

If AENCF is:

> 0.902 MeV,

then LBTL of 0.9579 is selected.

The lowest or smallest of the LBTLs are selected to be the final Lower Bound Tolerance Limit. [18] This will provide the most conservative approach for selecting a USL.



Figure 1. AENCF versus MCNP keff

The next step in calculating the USL is to determine the critical limit (CL). The CL is derived from the bias and uncertainties associated with the criticality code and modeling process. The CL equals the LBTL minus the sum of bias and uncertainties. The USL is equal to the CL minus any administrative margins. Figure 1 displays the graphical results of the USL search.

The USL for reprocessing is a limiting value of k_{eff} at which it the process will definitely be subcritical. This is to ensure that k_{eff} remains subcritical with all the allowances made for the bias and uncertainty in the calculation model as well as an administrative criticality safety margin.

An administrative criticality safety margin is determined by evaluating the validation results, the conservatisms in the calculation model, the likelihood of abnormal conditions, system sensitivity, and knowledge of neutron physics. Each one of these characteristics has applicability for analysis of possible situations that can occur before, during, or after reprocessing. A typical numerical value of -0.05 is selected. [18]

The average energy of the neutrons causing fission and the average neutron lethargy causing fission will indicate the spectrum of the benchmark. Table 2 shows the comparable benchmarks.

Benchmark	AENCF	EALF	Neutron Spectra
Special -Metal-Fast 001	1.28 M eV	1.33 MeV	96.7% fast
Special -Metal-Fast 002	1.28 MeV	1.33 MeV	96.8% fast
Special -Metal-Fast 003	0.838 MeV	0.838 MeV	94.4% fast

Table 2. AENCF and EALF of the benchmarks.

Once the range of parameters has been matched up with the range of applicability, then the next step will be to calculate the critical limit. The

uncertainty was calculated by squaring the standard deviation from the MCNP output, then summing the sigmas together, and then finally taking the square root of the sum.[23]

Uncertainty = $\sqrt{\sum \sigma^2 + \sigma^2}$..., σ = standard deviation

The uncertainties range from 0.00006 and 0.00013. Selecting the larger bias of 0.00013 will ensure a conservative calculation. The CL = LBTL – sum of bias and uncertainties = 0.9579 - 0.00013 = 0.9578.

The USL is equal to the CL minus the administrative margin (0.05). The final USL will be 0.9078. In order to ensure a subcritical system with the current set of benchmarks, in the fast spectrum, the k_{eff} needs to be less than 0.9078 for reprocessing.

ENDF/B-VII Data

In order to commence the research, three things must occur. First, an understanding of the ENDF file format must occur and then obtain the correct ENDF files for the eight identified isotopes. Second, the ENDF files will need to be converted into ACE tables by NJOY. Lastly, the MCNP code will be used to calculate the criticality levels of the benchmark models to determine reactivity changes.

One of the first things to understand is the file structure for ENDF tapes. ENDF data is collected by experimentation and verified by calculations. This is the starting point for creating new cross sections for MCNP. [6]

The current format is called ENDF6/B, version VII. The ENDF-format libraries are files of nuclear data that describe nuclear reaction cross sections, the distributions of energy and angle of reaction products, the various nuclei produced during nuclear reactions, the decay modes and product spectra resulting from the decay of radioactive nuclei, and the estimated errors in these quantities. The ENDF tapes allow calculations of decays and the transport of neutrons, photons, and charged-particles.

ENDF tapes are written in plain text, and formatted in ASCII text file. The ENDF libraries have a code structure that is determined by tape (MT), material (MAT), file (MF), and section (NSUB). A tape is a collection of materials (MAT), typically organized by ENDF libraries, (NLIB). A tape of materials often contains several different experimental data sets, usually from different labs around the world.[19] A library is a collection of evaluations from a specific evaluation group. A version (NVER) is a periodic update to an established library. The section library (NSUB) will determine what type of nuclear data one requires from the ENDF database. Some examples of NSUB are photo-nuclear data, radioactive decay data, spontaneous fission data, incident neutron data, thermal scattering data, and neutron induced fission product yields.

The file will be in presented in six columns with three identifier columns on the right to signify the MAT, MF/MT, and line number. The first six columns delineate the opening information on the isotope, the energy and cross-sections. There can be several MF/MTs in the same file. The delineation of some MT and MF sections are described in the Appendix.

The ever increasing scope of use for the ENDF-format data has led to a continual increase in the number and types of reactions that can be represented. Unfortunately, some materials have gaps in the ENDF database, and the NJOY-required MFs and MTs are missing. This produces crashes in the NJOY code, and resulting created cross sections are invalid. Troubleshooting of the ENDF file is required to be able to understand which MT or MF is missing, and then conduct a replacement with an identical isotope from another data source like other ENDF, JEF, or JENDL data files.

NJOY 99.259 Program

The NJOY Nuclear Data Processing System is used to convert evaluated nuclear data in ENDF format into forms useful for applications. [20] It is used by only a few specialists, and therefore needs to be researched carefully to ensure proper data in will equal correct information out. Its applications range from nuclear reaction theory, resonance theory, or scattering theory on one side, and some knowledge of a variety of subjects: for example, particle transport codes, reactor core calculations, and radiation medicine. NJOY is a powerful tool for shaping nuclear data to the purpose for which it is needed. [7]

Like the ENDF file structure and format, NJOY has gone through many iterations to improve the output and reduce the uncertainties in the calculations. The current version is 99.259. This version was used in generating all the cross-sections for the Monte Carlo N-Particle (MCNP) calculations.

NJOY was sent as source code from Radiation Safety Information

Computational Center (RSICC) and compiled in FORTRAN 95 format using G95, to make an executable program. The main executable file "njoy.exe" directs the flow of ENDF data through the specified modules and subroutines. NJOY is used in a DOS window, and is executed from a batch file that calls to a text file for which modules to use. Not all modules in NJOY will be discussed because they are not all applicable to processing cross-sections for MCNP criticality safety studies.

Before NJOY is run, the required sections of the ENDF tape are downloaded from BNL's website, the National Nuclear Data Center, to be saved into an ASCII file. In order to run NJOY, a batch file is created in a text editor that is run from DOS. [20] The first line of the batch file is a command to copy the ENDF tape to a randomly "numbered" tape. The second line is a call to the program to run the "dat" file that has the module decks. The "dat" file is created in a text editor as well. The third line is to copy the output of the NJOY program into a named text file. There are several other tapes created, but those will be discussed later, and they are determined by the modules that are run. For a review of what parameters went into the NJOY code, see the Appendix.



Figure 2. Cross Section Generation

When a cross section is generated, it is put into tabular form. One column of the table is for the energy level (in MeV) and the second column is for cross section (in barns). Starting at the top left corner of Figure 2, the isotope cross section decreases as temperature or energy level increases. It is roughly a 1/v relationship, until the resonance region is encountered. The resonance region has many energy points and probabilities, due to the numerous combinations of energy levels of the nucleons in the nucleus. As the energy increases after the resonance region, it continues to decrease until the threshold energy (~1 MeV) after which the cross section is less than two barns.[22]

Beta Effective

In order to calculate the realistic difference in reactivity of an isotope, a representative sample of that isotope needs to be placed in a reactor. Before the sample is placed in the center of the core, or gloryhole, a k_{eff} is measured with the gloryhole empty or voided. The sample isotope is then placed in the center and the increase in reactivity is then indirectly measured as the result of the increase in k_{eff} from the sample placement. In order to accurately measure the difference between a void and a replacement sample, the delayed neutron fraction is required to be known. [9]

A delayed neutron is one that has been emitted by an excited state of a nucleus immediately following beta decay. [22] The emission occurs when the decay leaves the daughter nucleus in an excited state that is above the neutron separation energy. Delayed neutrons account for approximately 0.75% of the neutron output from fission and this is an important aspect of controlling the increase in energy output of reactors. MCNP calculates the prompt neutron k_{eff}, but does not include the delayed neutron fraction. [21]

The value of beta effective is the weighted average of the total delayed neutron fractions of the individual types of fuel. Each total delayed neutron fraction value for each type of fuel is weighted by the percent of total neutrons that are fissionable isotopes.[11] Table 3 has the B_{eff} for the eight isotopes. [9]

 $\beta_{k}^{\text{AC}} = \frac{\sum_{i} \left(\sum_{g'} \mathcal{X}_{dk,g'} \beta_{g'}^{i} \mathcal{L}_{i,k}^{c} \sum_{g} \beta \Sigma_{fg,i} \beta_{g}^{i} \right)}{\sum_{i} \left(\sum_{g'} \mathcal{X}_{p,g'} (1 - \beta_{i}^{c}) \beta_{g'}^{i} \sum_{g} \nu \Sigma_{fg,i} \beta_{g}^{i} + \sum_{k} \sum_{g'} \mathcal{X}_{dk,g'} \beta_{g'}^{i} \mathcal{L}_{i,k}^{c} \sum_{g} \nu \Sigma_{fg,i} \beta_{g}^{i} \right)}$

Isotope	Beta Effective
U-235	0.0065
Np-237	0.00196
Pu-239	0.00276
Pu-240	0.00900
Pu-241	0.00157
Am-241	0.00130
Am-242m	0.00130
Am-243	0.00130
Cm-244	0.00204

Table 3. B_{eff} for the Higher Actinides

MCNP 5.1 Code

MCNP is a general-purpose <u>Monte Carlo N-Particle code that can be used for</u> neutron, photon, electron, or coupled neutron/photon/electron transport. Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis. The code treats an arbitrary threedimensional configuration of materials in geometric cells. [23] Pointwise cross-section data typically are used, although group-wise data is also available. For neutrons, all reactions given in a particular cross- section evaluation are accounted for. Thermal neutrons are described by both the free gas and $S(\alpha,\beta)$ models. For photons, the code accounts for incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, absorbtion in pair production with local emission of annihilation radiation, and bremsstrahlung.

Important standard features that make MCNP very versatile and easy to use include a powerful general source, criticality source, and surface source; both geometry and output tally plotters; a rich collection of variance reduction techniques; a flexible tally structure; and an extensive collection of cross-section data.

MCNP contains numerous flexible tallies: surface current & flux, volume flux (track length), point or ring detectors, particle heating, fission heating, pulse height tally for energy or charge deposition, mesh tallies, and radiography tallies.

An exhaustive search through all the criticality benchmark experiments from the IHCSEBE, combined with the criticality benchmark evaluation eliminated the majority of the experimental models. Only three benchmarks presented characteristics that were desirable for comparison with the range of applicability. The criticality evaluations for cross-section analysis will be performed by using MCNP for solving the neutron transport equation. [18]

The Monte Carlo method is based on tracking particles through their transport, including interactions such as scattering, fission and absorption, and
leakage. The probability curves bracketing these events are statistically sampled to describe their total activity. The cross sections for the various neutron interactions govern the reactions required for the criticality calculation at each step. The fission process is regarded as the birth event that separates generations of neutrons. A generation is the lifetime of a neutron from birth by fission, to loss by escape, parasitic capture, or absorption leading to fission. The average behavior of a group of neutrons is used to estimate the average behavior of the system (i.e., k_{eff}).

The KCODE capability of MCNP will be used to generate the k_{eff} term from the three benchmark models. This capability in MCNP will produce the fissions for counting neutron generations. For a review of what parameters went into the MCNP code, see the Appendix.

CHAPTER 3

METHODOLOGY

Criticality Benchmark Experiments

The selection of the three benchmarks was due to the similarities of the replacement isotopes and simple geometric configurations. Special-Metal-Fast-001 is a Dirty Jezebel, 20.1% Pu-240, with Pu-239 and Cm-244 replacements. Due to analyzing the isotopes from Np-237 to Cm-244, this benchmark is excellent for a comparative check. [9]

Special-Metal-Fast-002 is also a Dirty Jezebel, 20.1% Pu-240, with Pu-238 and Pu-239 replacements. The plutonium replacement is needed to verify reactivity worth of Pu-239. [9]

The last benchmark is Special-Metal-Fast-003, (Flattop). This is a core in a sphere within an outer sphere. There is a HEU core and Np-237 core, with either HEU or Pu outer casing. The HEU casing with the Np-237 core was selected. [9]

These three benchmarks will be able to provide data points for verification of the new cross-sections. Since fast spectrum cross sections were produced from NJOY then fast spectrum benchmarks are needed.

NJOY

The ENDF data was downloaded from BNL's website, (www.nndc.bnl.gov) for each isotope, utilizing the ENDF/B-VII family of data, from 2007. These are the latest nuclear data available. These data were stored in individual isotopeselected files, for all reactions.

The NJOY software was run for six temperatures (273.15 K, 281.15 K, 290.15 K, 300.15 K, 306.15 K, and 313.15 K). All eight isotopes had the six temperatures applied for a sum total of forty-eight NJOY runs. Each isotope, (at each of the six temperatures), will have generated an XSDIR output file, an ACE data library output, and a Postscript file to graphically view the new cross-sections.

Each of the XSDIR file outputs need to be modified to be added to MCNP's XSDIR file. The ACE data library needs to be moved to the MCNPDATA directory and the Postscript file needs to be converted for viewing, to ensure that the cross-section is continuous and covers the appropriate energy bands. Each isotope produced six ACE files, except for Am-242m. Missing ENDF/B-VII data prevented NJOY from producing all six temperature files; only three were made. The other forty five files were created and moved to the MCNPDATA directory and the XSDIR file was updated to reflect the changes. All created cross sections are presented graphically in Appendix I.

MCNP

The MCNP program will be utilized to calculate the reactivity worth of the replacement isotopes in the three benchmark models from the IHECSBE. This will be conducted by utilizing the KCODE card to measure k_{eff} on void and replacement models. The temperature is changed in small increments for each of the paired void and replacement runs in order to calculate the reactivity worth of the eight isotopes. This will be done for all three benchmarks.

Special-Metal-Fast-001 and -002 are both called Dirty Jezebels, due to the high loading of the Pu-240 isotope in the composition. The Dirty Jezebel benchmarks are simple spheres with a glory hole in the center for a void or replacement sample. The material of the Dirty Jezebel is a homogeneous mixture that contains 78.89 atomic weight % Pu-239, 20.1 atomic weight % Pu-240, and 1.01 atomic weight % Ga. The atomic weight percentage is determined by taking the isotopic weight, dividing it by the total mass of the compound, then multiplying it by 100. This will produce a percentage of all elements in a compound, normalized to a total of one.

The Special-Metal-Fast-001 benchmark had a glory hole of 0.3444 cm, as compared to the glory hole of 0.6437 cm in the Special-Metal-Fast-002 benchmark. Dirty Jezebel had an outer radius of 6.6595 cm.[9]

The Special-Metal-Fast-003 benchmark is called Flattop. It is a sphere in a sphere, with a 0.6921 cm glory hole. The material of the HEU core Flattop is a homogeneous mixture of 1.02 atomic weight % 234-U, 93.24 atomic weight % 235-U, and 5.74 atomic weight % 238-U. The replacement glory hole of Flattop

is 0.6921 cm. The outer radius of the inner sphere of enriched uranium was 6.1156 cm. The outer radius of the outer sphere of natural uranium was 24.1242 cm. [9]

The three IHECSBE benchmark models have the sample MCNP code in their respective appendices. For this research, the three benchmarks required to have calculated the six temperature-corrected cross sections, for the eight isotopes. Each benchmark needed to be computed separately with a void sample and a replacement sample. It will require ninety MCNP criticality runs for each benchmark, for a total of 270 individual perturbation runs.

The original three benchmark's MCNP program had 5,000 particles for 250 generations. The first 50 generations were disregard to allow the KCODE to start converging without averaging in the starting data . All of the MCNP kcode criticality runs originally commenced at a nominal k_{eff} of 1.0, to assist in converging the results faster. In effect, it is a best first guess for better convergence. The MCNP runs from the benchmark produced varying results, with a first sigma of +/- 0.00060 for all three benchmark models.

In an attempt to improve statistics for the three benchmarks, several iterations of increasing particles/generations and the total number of generations were run to improve statistics. Figure 3 shows that as the total particles increased; the standard deviations decreased. This produced an overall reduction in the first sigma from +/- 0.00060 to +/- 0.00008.



Figure 3. Standard Deviations versus Total Particles

The reason standard deviations are important is that BNL's ENDF/B data came in sixth decimal place accuracy.[6] NJOY will produce cross sections with sixth decimal place accuracy as well. MCNP creates k_{eff} to the fifth decimal place. It is necessary to increase the sigma to the fifth place in order to ensure the overall system uncertainty for computations will be mathematically accurate.

For the database, every run had to be organized and recorded under the appropriate isotope, temperature, void sample or replacement sample, and temperature. Each run was individually tailored for a different temperature that matched the surrounding materials. These temperatures ranged from 273.15 K to 313.15 K.

In order to make all the materials match the temperature of the cross sections, the use of the THTME and TMP cards is required. Individual cell energy level is calculated by multiplying Boltzmann's constant by the temperature of the material (in degrees Kelvin).

CHAPTER 4

FINDINGS OF THE STUDY

The newly created cross sections, as seen in the Appendix, were produced from NJOY, for all eight isotopes at all 6 temperatures. The quality check of comparision with NNDC's cross-section for all isotopes at 300.15 K was completed satisfactorily. This provided the approval to move forward with conducting the gloryhole void and replacement MCNP calculations.

Initial MCNP sensitivity runs for the Dirty Jezebel (r=0.3444cm) replacements disclosed just a few cents/gram difference between the eight target isotopes' calculations and the experimental models from the IHECSBE. In the benchmark, the experimental reactivity per gram versus calculated reactivity per gram at room temperature is presented in the below table. This is presented in Table 4 to show the qualification comparison of the IHECSBE data versus research data.

Sample	IHECSBE	IHECSBE	Research MCNP5
Isotope	Experimental Worth	Calculated Worth	Calculated Worth
	(cents/gram)	(cents/gram)	(cents/gram)
Pu-239	5.83	5.68+/-0.10	3.20826 +/- 0.00007
Cm-244	5.23	5.32+/-10	4.88074+/- 0.00007

Table 4. Reactivity-Worth Comparisons for Dirty Jezebel (0.3444 cm)

The second Dirty Jezebel (void r=0.6439cm) had the same increased histories, and longer generations applied in order to obtain better statistics. All eight isotopes had distinct increases from void to replacement k_{eff}. While the MCNP models are almost identical, the gloryhole size for the second Dirty Jezebel is roughly double the size from the first Dirty Jezebel model. The first Dirty Jezebel reactivity per gram changes did not form a linear regression line, and the data points were usually greater than one sigma from the regression line. Table 5 demonstrates the data from the second MCNP criticality runs.

Table 5. Reactivity-Worth Comparisons for Dirty Jezebel (0.6439 cm)

Sample	IHECSBE Experimental	IHECSBE	Research MCNP5
Isotope	Worth	Calculated Worth	Calculated Worth
	(cents/gram)	(cents/gram)	(cents/gram)
Pu-239	5.62	5.54+/-0.05	4.48366 +/- 0.00008

 Table 6. Reactivity-Worth Comparisons for Flattop

Sample	IHECSBE	IHECSBE	Research MCNP5	
Isotope	Experimental Worth	Calculated Worth	Calculated Worth	
	(cents/gram)	(cents/gram)	(cents/gram)	
Np-237	3.42+/-0.39	1.93+/-0.30	2.49730 +/- 0.00013	

The more complex MCNP model of the Flattop spheres also demonstrated increased k_{eff} from the void to replacement runs for each of the eight isotopes for all six temperatures. Table 6 presents the Flattop comparisons.

Even though the replacement samples for the Flattop model was calculated at 28.4g and the replacement sample for the second Dirty Jezebel was 22.9g, the smaller sample size of the Dirty Jezebel came in with higher reactivity per gram results than the Flattop. This may be attributed to the uranium reflector being less dense and allowing leakage of neutrons in the Flattop model.

The MCNP output data files present the information as k_{eff} and standard deviation. The division of void sample versus replacement sample provides the ability to differentiate how much reactivity is contributed from the isotope replacement.





These data can be graphically presented to demonstrate the even rise in k_{eff} from the void to the sample. This quality check demonstrates that the trend of calculations has resulted in k_{eff} increasing over all points from void sample to replacement sample as seen in Figure 4.

The three benchmarks combined data produced no significant increase in reactivity per gram per degree Kelvin (from 273.15 K to 313.15 K) for Np-237, Pu-240, Pu-241, and Am-241. The isotope Pu-239 showed a 0.75 cents/g increase and Am-243 showed an average of 2.5 cents per gram between the three benchmarks. Cm-244 showed an average of 2 cents per gram decrease in reactivity.



Figure 5. Reactivity Per Gram Diagram

A linear regression technique was used on the data to extract a flat "best fit curve" for the output of the three benchmarks, as shown on Figure 5. The regression lines do correlate with the data and look demonstrate an even trend with no overall increase or decrease in reactivity per gram for the change in temperature.

The Dirty Jezebel (0.34544 cm) MCNP model showed the worst statistics between void and replacement, while the larger sample in the Dirty Jezebel (0.6749 cm) gave larger or higher delta reactivity between void and replacement.

CHAPTER 5

RESULTS, CONCLUSIONS, AND RECOMMENDATIONS

Discussion of Results

The calculations of the eight isotopes for each of the six specified temperatures were successful, except for three of the temperatures of Am-242m. Void and replacement calculations were conducted, and then provided replacement reactivity per gram measurements for all eight isotopes in the fast spectrum. The data correlated with the IHECSBE, thus providing a quality check for the process. The first Dirty Jezebel model produced slightly erratic data for all the isotope replacement runs. It was roughly within three sigma of the other two models, but no discernable pattern could be determined for a best fit analysis. The second Dirty Jezebel and the Flattop model's data concurred with each other and provided a level of confidence that the information was correct.

A recommendation will be to numerically dismiss the data and trend analysis of the SMF-001 (Dirty Jezebel 0.3444cm) benchmark. This is a result of the first Dirty Jezebel's data points falling outside of one if not two sigma from the rest of the model's data for the other two benchmarks. While this area of uncertainty between the first model and the last two models is large and not able to be averaged into the other data, it does provide verification that the models are within a few digits of each other.

Another recommendation is to use all cross sections from the studied isotopes, and at the observed temperatures. The cross sections appear to have presented all the required data in the right format and generated effective criticality runs. The IHECSBE data and this research agree at many points for k_{eff} , reactivity per gram, and overall model behavior. Caution would be prudent in using the Am-242m isotope, due to missing ENDF/B-VII data that prevented creating more than the three cross sections at 273.15 K, 300.15 K, and 313.15 K.

Three of eight isotopes have demonstrated noticeable changes in reactivity per gram that can be utilized in future fast spectrum research. Pu-239, Am-243, and Cm-244 are the only isotopes that showed this change in reactivity for a change in temperature. This is required in order to be able to determine reactivity when conducting replacement experiments.

The trends and results of the eight isotopes are similar to the benchmarks. While the data is not exactly replicated, the statistical variances put the data within range. It was expected that the higher actinides would have slightly increasing changes in reactivity per gram to difference in temperature, but only 3 of 8 were reactive. This is beneficial in that reprocessing would not significantly change the k_{eff} of the aqueous solution for the fast spectrum. Further research is required to determine if the higher actinides are temperature sensitive in the thermal ranges.

Conclusions and Recommendations for Further Study

After correctly running NJOY to process ENDF nuclear data and then conducting MCNP KCODE runs for all the isotopes for the six temperatures, the cross section results are documented in the Appendix for all three models at 272.15 K and 313.15 K. All eight isotopes reviewed did not appear to change with the increase in temperature from 273.15 K to 313.15 K. The reactivity per gram graphs are documented in the Appendix. While the first Dirty Jezebel replacement model was not as predictable as the other two models, it did provide a quality check that the data was similar.

All eight isotopes should continue to be evaluated for performance characteristics in the thermal spectrum, in order to obtain a clearer picture of their behavior under all energy ranges. The individual thermal cross sections will then be evaluated in an aqueous solution, in order to simulate the reprocessing system.

Creating a NJOY multi-group fast and thermal cross section that will represent all eight isotopes will give indications of how the higher actinides will perform in combination with each other. The goal will be to conduct an experiment of all the actinides in a solution in the temperature range from 273.15 K to 313.15 K, that will satisfy the USL and demonstrate the rate at which reprocessing can occur.

The multi-group and individual cross-sections will be scheduled to be experimentally verified in the University of New Mexico's AGN-201 reactor. The recommendation is to obtain X grams of thermally sensitive isotope Y. This will

provide a validation of the cross-sections from NJOY and the AGN-201 model for MCNP.

Issues

BNL's ENDF data has changed several times since the start of this research a year ago. There were 300 K data available as well as the regular ENDF data, but they have been removed from the website. Am-242m is not currently fully structured. MT6 MF0 and MT2 MF 451 are missing from several isotopes, so NJOY fails on ACER verification for the double precision accuracy cross-section formation.

APPENDIX

COMPUTER CODE AND DATA

ENDF

The material files (MF) for each material have particular parameters, such as:

MF=1 contains descriptive and miscellaneous data,

MF=2 contains resonance parameter data,

MF=3 contains reaction cross sections vs energy,

MF=4 contains angular distributions,

MF=5 contains energy distributions,

MF=6 contains energy-angle distributions,

MF=7 contains thermal scattering data,

MF=8 contains radioactivity data

MF=9-10 contain nuclide production data,

MF=12-15 contain photon production data,

MF=23 Photo-atomic interaction cross sections

MF=27 Atomic form factors or scattering functions for photo-atomic

Interactions

MF=30-40 contain covariance data.

The MT section labels the individual parameters of each MF section. Sections are usually used to hold different reactions. For example:

MT=1 is the total cross section,

MT=2 is elastic scattering,

MT=3 (z, non-elastic) Nonelastic neutron cross section. Sum of MT=4,

5, 16-18, 22-26, 28-37, 41-42, 102-116

MT=4 (z,n) Cross section for the production of one neutron in the exit channel. Sum of the MT=50-91.

MT=5 (z,anything) The cross section for the sum of all reactions not given explicitly in another MT number.

MT=10 (z,continuum) Total continuum cross section. This sum cross section includes all continuum reactions and excludes all others MT=16 is the (n, 2n) reaction.,

MT=18 is fission,

MT=102 is radiative capture, and many others.

NJOY

NJOY.exe Batch File

copy ENDFtext.txt tape20 njoy<thesis237Np.dat copy output output.txt

NJOY.exe Input Dat File

moder 20 - 21 reconr -21 -22 'thesis test 4'/ 9346 0 0/ .001/ 0/ broadr -21 -22 -23 9346 6 0 0/ .001/ 273.15 281.15 290.15 300.15 306.15 313.15/ 0/ unresr -21 -23 -24 9346 6 9 1 273.15 281.15 290.15 300.15 306.15 313.15/ 1e10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/ 0/ heatr -21 -24 -25 34/ 9346 12/ 302 303 304 318 401 402 442 443 444 445 446 447/ thermr 0 - 25 - 26 0 9346 16 6 1 0 1 221 2/correct this line 273.15 281.15 290.15 300.15 306.15 313.15/ .001 5/ gaspr -21 -26 -27 purr -21 -27 -28 9346 6 9 20 64 1 0 / 273.15 281.15 290.15 300.15 306.15 313.15 /

```
1e10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/
0/
acer
-21 -28 0 29 30
1 0 1 .07 0/ fast data at 273.15K
'thesis test 4'/
9346 273.15/
1/
1
acer
0 29 31 32 33
7 1 1/
'thesis test 4'/
viewr
31 59/
stop
```

NJOY Sample File Explanation

The following is an example of an input NJOY batch file:

copy ENDFtext.txt tape20

njoy<thesis237Np.dat

copy output output.txt

One of the first modules needing to be addressed is the MODER module. This module is not required, but is necessary if computational speed is desired. It will translate the ENDF tape from ASCII format to a special blocked-binary format. If MODER is used at the beginning, then it is also needed on the end of the input deck to convert the blocked-binary back to ASCII. The first number after MODER is the original tape into which the ENDF file was copied. The second number is the tape number into which the ASCII tape is being copied, and the sign is negative to show the conversion from ASCII to blocked-binary.

moder

20 - 21

The next module that is called, is RECONR. This module can conduct several operations at once. RECONR builds a union grid from linear interpolation of the ENDF data. First, the module calls the tape that is first named on the second line. The output of the module is the second number on the first card, which is called the PENDF, or pointwise ENDF tape. The second card is the title of the project/reason the module is being run. The third card is the material, number of cards for new MF1, and number of energy grid points to be added. When in

doubt, use defaults! The fourth card is the error tolerance, usually set at .001. Card number five is set to zero to terminate the module.

reconr -21 -22 'thesis test 4'/ 9346 0 0/ .001/ 0/

The third module that is called for is the BROADR module. After the pointwise cross sections are generated from RECONR, BROADR adds temperature dependence in accordance with the relative difference in velocities of the material and the neutron, alpha=M/(2kT).

On card one. the BROADR module, pulls in the thermal unbar from tape number 21 and the PENDF data from tape number 22. The output PENDF of BROADR will be written to tape number 23, all are negative to show calculations are being done in blocked-binary. Card two is the material number and the number of temperatures for the material to be analyzed. Card three is the error tolerance. Card four is the temperatures (in Kelvin). Card five is the termination card.

broadr

-21 -22 -23 9346 3 0 0/ .001/

273.15 300.15 313.15/

0/

The next module is UNRESR. At the higher energies, resonances get so close together that they cannot be effectively separated. Instead of giving individual resonances with separate energies and characteristic widths, ENDF-format evaluations give average values for the resonance spacing and the various characteristic widths, together with the probability distributions (PURR) needed to describe the quantities.

The first card is calling ENDF data from tape 21, to request ENDF data. It is also calling the PENDF data from BROADR, and it is outputting the updated PENDF data into tape 24. The second card stipulates the material, the number of temperatures, the number of sigma zeros, and the output print options. The third card is the temperatures, while the fourth card gives the sigma zeros. The last card is a termination card.

unresr -21 -23 -24 9346 3 9 1 273.15 300.15 313.15/ 1e10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/ 0/

HEATR is the next module and it computes KERMA heating and radiation damage energy production. These details are added to the pointwise union grid created by the last module.

The cards for HEATR are simple. The first card is for ENDF and PENDF tape inputs, with the PENDF output going to tape 25. Tape 34 is for graphical output check. The second card is for the material and the number of partial KERMAS to calculate. The third card is to specify the partial KERMAs to calculate.

heatr

-21 -24 -25 34/

9346 12/

302 303 304 318 401 402 442 443 444 445 446 447/

THERMR is the next module. THERMR generate neutron scattering cross sections and point-to-point scattering kernels in the thermal range, and add pointwise scattering cross sections and scattering matrices to an existing PENDF tape.

The first card specifies the input ENDF (for MF7 data) and input PENDF tapes, and the output PENDF file to tape 26. The second card is the material with the MF7 data, the material on the PENDF tape, number of angles, number of temperatures, inelastic option, elastic option, number of principal atoms, inelastic MT number, and print option. The third card is the temperatures. The fourth card is the tolerance and max E.

thermr

0 - 25 - 26

0 9346 16 3 1 0 1 221 2/correct this line 273.15 300.15 313.15/ .001 5/

The GASPR module will add charged-particle production cross sections to the PENDF tape. While this is not important for solid material MCNP transport code, it is vital for solutions, and that will be useful when calculating reprocessing simulations. The GASPR module is simple; the first card specifies the input ENDF and PENDF tapes, and the output PENDF file to tape 27.

gaspr

purr

-21 -26 -27

The bondarenko moments (for convergence) and probability tables are added to the PENDF tape by the PURR module. The first card specifies the input ENDF and PENDF tapes, and the output PENDF file to tape 28. The second card indicates the material, the number of temperatures, the number of sigma zeros, number of probability bins, number of resonance ladders, print option, and number of energy points (0=all). The third card is the specified temperatures, and the fourth card is the numerical value of the sigma zeros. The fourth card is a termination card.

> -21 -27 -28 9346 3 9 20 64 1 0 / 273.15 300.15 313.15 / 1e10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1/ 0/

The ACER module is the transition between calculating the data from NJOY and making it available for MCNP use. After all the data points have been added

to the PENDF tape, it is ready for conversion to a format readable by MCNP. The first card specifies the input ENDF, PENDF and GENDF tapes. The second half of the first card is the trial output ACE tape and trial output line for MCNP's xsdir file. The second card on this module is specifying that it is fast data, no print, ACE format type 1, NN=07 (from the zaid. NNc), and the number of iz/aw pairs to read in(0). The third card is the label. The fourth card is the material and temperature for this ACE library. The fifth card is a default to use the new law 61 cumulative angle distributions.

acer

-21 -28 0 29 30 1 0 1 .07 0/ fast data at 273.15K 'thesis test 4'/ 9346 273.15/ 1 /

1

The ACER module is run a second time to clean up, verify, and finalize the ACE library. The first card calls for no ENDF file. It then calls for the output of the last ACER module, tape 29. The third number is the plotting output tape 31 for VIEWR, The second half of the first card is the final output ACE tape 32 and final output tape 33 for MCNP's xsdir file. The second card is to specify that this is a check of an ACE type 1 tape, max printing option, and the output is a type 1 ACE library. The fourth card is the label.

acer

0 29 31 32 33

7 1 1/

'thesis test 4'/

Tape 33 will need to be modified so that it is readable by MCNP. Ensure that the line is placed in the xsdir file, right after the AWR listings. Verify that the NN is replaced by two numbers that do not conflict with any other library in the xsdir file. Replace the file name with the ACE library name that is selected. Replace the word "route" with the number 0. Tape 32 will be the final ACE library output. Open up tape 32 and check that the zaid.NNc has the same NN as specified in the xsdir file. Remember to name the tape 32 as the same name that you replaced with the new "filename" word from the xsdir file. If this is not done, MCNP will not be able to access or find the new ACE library.

93237.NNc 235.011800 filename route 1 1 536245 0 0 2.354E-08 ptable The last module is VIEWR. This will take the output of the ACER module and convert it into a Postscript file called tape 59.

viewr

31 59/

















MCNP

MCNP Sample Input Explanation

The three MCNP programs are similarly written. The first section contains the cell cards that define the title, material, space, boundaries, density, and importance. For example:

Special Metal Fast One- DJ Replacement

c cell number mat number density in/out importance \$comments

с 1	1	-0.1e-9	-1	imp:n=1	\$ void
1	1	-13.67	-1	imp:n=1	\$ sphere filled
2	2	0.04055292	1 -2	imp:n=1	
3	0		2	imp:n=0	

The second section identifies the surface cards that make up the cell cards. The surface cards make planes or geometric shapes that make up the inside and outside boundary of of an object.

- 1 so 0.3444
- 2 so 6.6595

The third section defines that materials, sources, tallies, time, temperature, and print options. The material card is structured to state the isotopic mixture or density. The source card will identify the energy, starting location, and direction of the radioactive source. The KCODE card will state the particles per generation, the number of generations, initial k_{eff} , and the number of generations to throw away prior to averaging.
The "fcl:n 1 1 0" card forces one collision for every particle entering into cell 1. The "f24:n 1" card (track length k_{eff} neutron tally card) is used to modify the track length flux tally in cell 1 to produce a track length k_{eff} for cell 1. The "fm24 -1. 1 -6 -7" card (tally multiplier card) multiplies the track length tally, previously specified by the f24:m 1 card, by the cell atom density, and by sigma f, and by nu for material 1. The quantity sigma f1 is k_{eff} when integrated over all energies. The "sd24 1" card prevents division by the cell volume, which results in an integral tally. The "e24" card (tally energy card) defines the energy bins into which the tallies are tracked. The "cf24 1" card specifies that a separate tally is maintained for all particles entering material 1. The print card specifies what tables to print, (all, none or specified ones). The thtme and tmp cards work together to specify cell card temperature. [7]

m1 95242.96c -13.67
m2 94239.96c 0.029934
94240.96c 0.0078754
94241.96c 0.0012146
94242.50c 0.00015672
31000.50c 0.0013722
kcode 5000 1.0 50 250
sdef pos 0 0 0 rad d1
si1 0.3444
fcl:n 1 0 0
phys:n j 20.

thtme 0

c tmp0 2.353734e-8 2.353734e-8 2.353734e-8 \$273.15K .94c c tmp0 2.423E-08 2.423E-08 2.423E-08 \$ 281.15K .91c c tmp0 2.500E-08 2.500E-08 2.500E-08 \$290.15 .92c c tmp0 2.58639e-8 2.58639e-8 2.58639e-8 \$ 300.15K .95c c tmp0 2.638E-08 2.638E-08 2.638E-08 \$ 306.15K .93c tmp0 2.698414e-8 2.698414e-8 2.698414e-8 \$313.15K .96c f24:n 1 fc24 fm24 -1. 1 -6 -7 sd24 1. e24 1-5 1-4 1-3 1-2 .1 .5 1 18i 20 cf24 2 print

MCNP is well documented in many publications. This is a terse presentation for a quick refresher.

MCNP5.exe Input File #1

Special Metal Fast One- DJ Replacement c1 1 -0.1e-9 -1 imp:n=1 \$ void 1 1 -13.67 -1 imp:n=1 \$ sphere filled 2 2 0.04055292 1-2 imp:n=1 3 0 2 imp:n=0 1 0.3444 SO 2 6.6595 SO m1 95242.96c -13.67 m2 94239.96c 0.029934 94240.96c 0.0078754 94241.96c 0.0012146 94242.50c 0.00015672 31000.50c 0.0013722 kcode 5000 1.0 50 250 sdef pos 0 0 0 rad d1 0.3444 si1 fcl:n 100 phys:n j 20. thtme 0 c tmp0 2.353734e-8 2.353734e-8 2.353734e-8 \$ 273.15K .94c c tmp0 2.423E-08 2.423E-08 2.423E-08 \$281.15K.91c c tmp0 2.500E-08 2.500E-08 2.500E-08 \$290.15 .92c c tmp0 2.58639e-8 2.58639e-8 2.58639e-8 \$300.15K .95c c tmp0 2.638E-08 2.638E-08 2.638E-08 \$306.15K .93c tmp0 2.698414e-8 2.698414e-8 2.698414e-8 \$ 313.15K .96c f24:n 1 fc24 fm24 -1.1-6-7 sd24 1. e24 1-5 1-4 1-3 1-2 .1 .5 1 18i 20 С cf24 2

print

MCNP5.exe Input File #2

Special Metal Fast 2 replacements measurement in DJ c 1 1 -0.1e-9 -1 imp:n=1 \$ void 1 1 -13.5 -1 imp:n=1 \$ sphere filled 2 2 0.04055292 1 -2 imp:n=1 3 0 imp:n=0 2 1 0.6439 SO 2 6.6595 SO m1 96244.96c -13.5 m2 94239.96c 0.029934 94240.96c 0.0078754 94241.96c 0.0012146 94242.50c 0.00015672 31000.50c 0.0013722 kcode 5000 1.0 50 250 sdef pos 0 0 0 rad d1 si1 0.6439 fcl:n 110 phys:n j 20. thtme 0 c tmp0 2.353734e-8 2.353734e-8 2.353734e-8 \$273.15K .94c c tmp0 2.423E-08 2.423E-08 2.423E-08 \$281.15K .91c c tmp0 2.500E-08 2.500E-08 2.500E-08 \$290.15 .92c c tmp0 2.58639e-8 2.58639e-8 2.58639e-8 \$300.15K .95c c tmp0 2.638E-08 2.638E-08 2.638E-08 \$306.15K .93c tmp0 2.698414e-8 2.698414e-8 2.698414e-8 \$ 313.15K .96c f24:n 1 fc24 fm24 -1.1 -6 -7 sd24 1. e24 1-5 1-4 1-3 1-2 .1 .5 1 18i 20 cf24 1 print

MCNP5.exe Input File #3

Special Metal Fast Three- Replacements in HEU flattop 1 -0.1e-9 c 1 -1 imp:n=1 \$ void -13.5 1 1 -1 imp:n=1 \$ filled sphere 2 0 1 - 2 imp:n=1 3 2 0.0476662 2 -3 imp:n=1 4 3 0.0480675 3-4 imp:n=1 5 0 4 imp:n=0 1 so 0.6921 2 so 0.7266 3 so 6.1156 4 so 24.1242 m1 96244.96c -13.5 m2 92234.50c 0.00048869 92235.50c 0.044482 92238.50c 0.0031842 m3 92235.50c 0.00035050 92238.50c 0.047717 kcode 5000 1.0 50 250 sdef pos 0 0 0 rad d1 thtme 0 c tmp0 2.353734e-8 2.353734e-8 2.353734e-8 2.353734e-8 2.353734e-8 \$273.15K .94c c tmp0 2.423E-08 2.423E-08 2.423E-08 2.423E-08 2.423E-08 \$281.15K.91c c tmp0 2.500E-08 2.500E-08 2.500E-08 2.500E-08 2.500E-08 \$290.15.92c c tmp0 2.58639e-8 2.58639e-8 2.58639e-8 2.58639e-8 2.58639e-8 \$ 300.15K .95c c tmp0 2.638E-08 2.638E-08 2.638E-08 2.638E-08 2.638E-08 \$ 306.15K .93c tmp0 2.698414e-8 2.698414e-8 2.698414e-8 2.698414e-8 2.698414e-8 \$313.15K .96c si1 6.1156 fcl:n 10110 f24:n 1 fc24 fm24 -1.1-6-7 sd24 1. e24 1-5 1-4 1-3 1-2 .1 .5 1 18i 20 cf24 1

print

	Townshing (14)				- 4-1-1
Isotope	[Temperature(K)	Dirty Jezebel3cm	stddev	replacement keff	stddev
Base stats	K		0.00004	4 00040	0.00005
237Np	273.15	0.99973	0.00004	1.00012	0.00005
	281.15	0.99960	0.00005	0.99973	0.00005
	290.15	0.99939	0.00005	0.99979	0.00005
	300.15	0.99974	0.00005	0.99990	0.00005
	306.15	0.99956	0.00005	0.99974	0.00005
	313.15	0.99973	0.00005	0.99992	0.00005
239Pu	273.15	0.99971	0.00005	1.00012	0.00005
		0.99957	0.00005	0.99988	0.00005
	290.15	0.99964	0.00005	0.99994	0.00005
	300.15	0.99976	0.00005	1.00006	0.00005
	306.15	0.99950	0.00005	0.99988	0.00005
	313.15	0.99973	0.00005	1.00019	0.00005
240Pu	273.15	0.99963	0.00005	0.99999	0.00005
	281.15	0.99962	0.00005	0.99967	0.00005
	290.15	0.99942	0.00005	0.99979	0.00005
	300.15	0.99972	0.00005	1.00011	0.00005
	306.15	0.99958	0.00005	0.99976	0.00005
	313.15	0.99972	0.00005	0.99996	0.00005
241Pu	273.15	0.99977	0.00005	1.00008	0.00005
	281.15	0.99955	0.00005	0.99991	0.00005
	290.15	0.99947	0.00005	0.99996	0.00005
	300.15	0.99969	0.00005	1.00006	0.00005
	306.15	0.99950	0.00005	0.99993	0.00005
	313.15	0.99969	0.00005	1.00010	0.00005
241Am	273.15	0.99978	0.00005	0.99982	0.00005
	281.15	0.99955	0.00005	0.99972	0.00005
	290.15	0.99962	0.00005	0.99974	0.00005
	300.15	0.99975	0.00005	0.99987	0.00005
	306.15	0.99941	0.00005	0.99979	0.00005
	313.15	0.99978	0.00005	0.99984	0.00005
242mAm	273.15	0.99974	0.00005	1.00008	0.00005
	300.15	0.99968	0.00005	1.00005	0.00005
	313.15	0.99974	0.00005	1.00009	0.00005
243Am	273.15	0.99967	0.00005	0.99982	0.00005
	281.15	0.99945	0.00005	0.99965	0.00005
	290.15	0.99960	0.00005	0.99970	0.00005
	300.15	0.99969	0.00005	0.99989	0.00005
	306.15	0.99949	0.00005	0.99969	0.00005
	313.15	0.99964	0.00005	0.99988	0.00005
244Cm	273.15	0.99959	0.00005	0.99991	0.00005
	281.15	0.99950	0.00005	0.99978	0.00005
	290.15	0.99953	0.00005	0.99976	0.00005
	300.15	0.99962	0.00005	0.99986	0.00005
	306.15	0.99953	0.00005	0.99979	0.00005
	313.15	0,99977	0.00008	0.99984	0.00005

MCNP output in table form for first Dirty Jezebel (r=0.3444cm)

	Void Keff				
Isotope	Temperature(K)	Dirty Jezebel6cm	stddev	replacement keff	stddev
Base stats	K	void Keff		· · · · · · · · · · · · · · · · · · ·	
237Np	273.15	0.99836	0.00006	0.99958	0.00006
	281.15	0.99811	0.00006	0.99937	0.00006
	290.15	0.99811	0.00006	0.99934	0.00006
	300.15	0.99815	0.00006	0.99953	0.00006
	306.15	0.99799	0.00006	0.99946	0.00006
	313.15	0.99833	0.00006	0.99955	0.00006
239Pu	273.15	0.99824	0.00006	1.00072	0.00006
	281.15	0.99795	0.00006	1.00057	0.00006
	290.15	0.99796	0.00006	1.00070	0.00006
	300.15	0.99820	0.00006	1.00072	0.00006
	306.15	0.99814	0.00006	1.00064	0.00006
	313.15	0.99831	0.00006	1.00073	0.00006
240Pu	273.15	0.99829	0.00006	0.99976	0.00006
	281.15	0.99799	0.00006	0.99953	0.00006
	290.15	0.99813	0.00006	0.99954	0.00006
	300.15	0.99828	0.00006	0.99970	0.00006
	306.15	0.99814	0.00006	0.99969	0.00006
	313.15	0.99831	0.00006	0.99973	0.00006
241Pu	273.15	0.99813	0.00006	1.00055	0.00006
	281.15	0.99805	0.00006	1.00027	0.00006
	290.15	0.99812	0.00006	1.00026	0.00006
	300.15	0.99819	0.00006	1.00048	0.00006
	306.15	0.99804	0.00006	1.00029	0.00006
	313.15	0.99811	0.00006	1.00056	0.00006
241Am	273.15	0.99825	0.00006	0.99931	0.00006
	281.15	0.99806	0.00006	0.99919	0.00006
	290.15	0.99814	0.00006	0.99918	0.00006
	300.15	0.99832	0.00006	0.99936	0.00006
	306.15	0.99803	0.00006	0.99918	0.00006
	313.15	0.99816	0.00006	0.99930	0.00006
242mAm	273.15	0.99820	0.00006	1.00058	0.00006
	300.15	0.99813	0.00006	1.00060	0.00006
	313.15	0.99828	0.00006	1.00048	0.00006
243Am	273.15	0.99827	0.00006	0.99914	0.00006
	281.15	0.99805	0.00006	0.99895	0.00006
	290.15	0.99803	0.00006	0.99895	0.00006
	300.15	0.99820	0.00006	0.99914	0.00006
	306.15	0.99810	0.00006	0.99891	0.00006
	313.15	0.99823	0.00006	0.99915	0.00006
244Cm	273.15	0.99821	0.00006	0.99963	0.00006
	281.15	0.99807	0.00006	0.99952	0.00006
	290.15	0.99804	0.00006	0.99943	0.00006
	300.15	0.99821	0.00006	0.99972	0.00006
	306.15	0.99804	0.00006	0.99947	0.00006
	313.15	0.99821	0.00006	0.99962	0.00006

MCNP output in table form for first Dirty Jezebel (r=0.6439cm)

		Void Keff			
Isotope	Temperature(K)	Flattop	stddev	replacement keff	stddev
Base stats	ĸ	void Keff			
237Np	273.15	0.99819	0.00006	0.99959	0.0008
	281.15	0.99826	0.00008	0.99951	0.00008
	290.15	0.99822	0.00008	0.99961	0.00010
	300.15	0.99823	0.00008	0.99957	0.00008
	306.15	0.99828	0.00008	0.99966	0.00008
	313.15	0.99836	0.00008	0.99962	0.0008
239Pu	273.15	0.99826	0.00006	1.00129	0.00006
	281.15	0.99821	0.00008	1.00105	0.00008
	290.15	0.99810	0.00007	1.00101	0.00008
	300.15	0.99823	0.00008	1.00009	0.00008
	306.15	0.99820	0.00008	1.00119	0.0008
	313.15	0.99826	0.00008	1.00115	0.00008
240Pu	273.15	0.99825	0.00006	0.99984	0.00008
	281.15	0.99826	0.00007	0.99997	0.0008
	290.15	0.99828	0.00007	0.99988	0.00008
	300.15	0.99828	0.00007	0.99973	0.00008
_	306.15	0.99828	0.00007	0.99979	0.00008
	313.15	0.99828	0.00007	0.99973	0.00008
241Pu	273.15	0.99816	0.00006	1.00125	0.00008
	281.15	0.99815	0.00007	1.00112	0.00008
	290.15	0.99815	0.00007	1.00112	0.00009
	300.15	0.99820	0.00007	1.00101	0.00008
	306.15	0.99825	0.00008	1.00099	0.00008
	313.15	0.99826	0.00007	1.00084	0.00008
241Am	273.15	0.99818	0.00006	0.99924	0.00008
	281.15	0.99811	0.00008	0.99927	0.00008
	290.15	0.99824	0.00008	0.99899	0.00010
	300.15	0.99829	0.00008	0.99917	0.00008
	306.15	0.99825	0.00008	0.99923	0.00008
	313.15	0.99815	0.00008	0.99933	0.00008
242mAm	273.15	0.99821	0.00006	1.00113	0.00008
	300.15	0.99830	0.00008	1.00088	0.00007
	313.15	0.99813	0.00008	1.00102	0.00008
243Am	273.15	0.99825	0.00006	0.99903	0.00008
	281.15	0.99812	0.00008	0.99896	0.00008
	290.15	0.99830	0.00008	0.99893	0.00009
	300.15	0.99824	0.00007	0.99898	0.00008
	306.15	0.99824	0.00007	0.99898	0.00007
	313.15	0.99834	0.00008	0.99906	i 0.00008
244Cm	273.15	0.99818	0.00006	0.99972	0.00008
	281.15	0.99832	0.00008	0.99984	0.0008
	290.15	0.99832	0.00008	0.99959	0.00009
	300.15	0.99821	0.00008	0.99973	0.00008
	306.15	0.99831	0.00008	0.99992	0.00008
	313.15	0.99818	0.00008	0.99967	0.00008

MCNP output in table form for Flattop (r=0.6921cm)





Temperature (K)





Temperature (K)



Reactivity per Gram



Reactivity per Gram



Am-243 Reactivity per Gram



Readivity per gram

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