COUPLED DIFFERENTIAL AND INTEGRAL DATA ANALYSIS FOR IMPROVED UNCERTAINTY QUANTIFICATION OF THE $^{63,65}$CU CROSS-SECTION EVALUATIONS

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Coupled Differential and Integral Data Analysis for
Improved Uncertainty Quantification of the $^{63,65}$Cu Cross
Section Evaluations

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Abstract

A new methodology has been developed that couples differential cross section data evaluation with integral benchmark analysis for improved uncertainty quantification. The new methodology was applied to the two new copper evaluations and resulted in an improved evaluation with smaller covariance data. Copper is a structural material in many nuclear applications, particularly those dealing with criticality safety. The current standard for the resonance evaluation of the two copper isotopes, $^{63,65}$Cu, has been determined to result in poor modeling performance. Therefore a new resonance evaluation of the two copper isotopes is vital to nuclear criticality safety applications. Performing a new resolved resonance region evaluation for copper has served as a backdrop to this work on developing new techniques for resolved resonance region evaluation. For the new evaluations, experimental cross section measurements have been carried out in the thermal energy region where no experimental data had previously been measured. Along the way, an automated routine was developed to aid with the determination of the quantum angular momentum of newly identified resonances. The impact of differential scattering cross sections with respect to angle was determined in the benchmarking process. The implications of the study of the impact of differential cross sections on criticality suggest a necessity for detailed treatment of the angular distributions during the evaluation process, as well as temperature broadening of the angular distributions for simulation applications. The formalism for temperature broadening of angular distributions has been derived and tested. The new evaluations were compared against the current ENDF/B-VII.1 standard on a set of 23 criticality safety benchmark models and displayed improved performance. In the new methodology developed for coupling of the differential and integral data evaluation, resonance parameters are directly and systematically adjusted based on feedback from integral benchmark experiments. Coupling this feedback directly to the resonance parameters gives the new method the advantage of implicitly adjusting all of the cross sections simultaneously, including the double differential cross
sections. Based on integral feedback, the new methodology provides a way of updating the reported covariance of the resolved resonance region to reflect true state of knowledge.

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Chapter 1

Introduction

Over the past decade, large discrepancies between the computed and the experimentally recorded $k_{eff}$ of criticality safety benchmark experiments containing copper were noticed by the nuclear data and criticality safety community [23]. The most notable of these benchmarks is the set of Highly Enriched Uranium METal fuels with copper reflectors from the Zeus experiment, that is, HEU-MET, from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [5].

In the world of nuclear fission, copper is used as a minor structural material in many nuclear facilities. In fact, a quick search through the ICSBEP handbook reveals that copper is significant in 32 of the 586 evaluated criticality safety benchmarks and found in 1084 cases out of 4708 documented cases in ICSBEP. Copper is also an important structural component in Scandinavian spent fuel casks [22].

Copper is an important heat sink material for fusion power reactors and is also used for diagnostics, microwave wave guides and mirrors in the International Thermonuclear Experimental Reactor (ITER). The available nuclear data evaluations for stable $^{63,65}$Cu isotopes are not as consistent as required for accurate activation and particle transport calculations in fusion systems. Consistent and correct data evaluations are of high priority for applications to the International Fusion Materials Irradiation Facility (IFMIF) where the equipment must resist high energy particle irradiation. As a prerequisite the general purpose neutron data files must include all information required for a wide spectrum of nuclear analyses including simulations...
of neutrons and the assessment of the nuclear heating, damage and gas production. The more accurate nuclear data is an important element of quality assured analyses for the design and optimization of all fusion related facilities including ITER and its planned successor reactor, DEMOnstration Power Plant (DEMO), as well as the IFMIF neutron source.

The neutron cross section of the copper isotopes is also important to the astrophysics community. The two stable isotopes of copper lie along the beta-decay valley of stable isobars involved in the s-process or slow-neutron-capture-process. In the s-process, a nucleus captures a neutron and then beta-decays to produce heavier isotopes. The s-process occurs in stars and is responsible for the creation of approximately half of the stable isotopes heavier than iron and therefore plays an important role in the galactic chemical evolution. Improving the evaluation copper evaluations will aid astrophysicists in reduce the uncertainty in current models of the universe.

In order to improve the systematic procedure for requesting nuclear data for criticality safety applications, the Department of Energy (DOE) has developed a mechanism by which criticality safety practitioners are able to identify their data needs. To undertake this responsibility, the DOE has established the Nuclear Data Advisory Group (NDAG). NDAG maintains and constantly updates lists of materials that are considered important for applications in nuclear criticality safety. Surveys of the status of existing nuclear data included in the listing are made. The results from this investigation are reported, and ranks of the most-needed evaluated nuclear data are issued. In particular, the two copper isotopes \(^{63,65}\text{Cu}\) were identified on this list as "Important for measurement and evaluation in the next five years." [26]

In general, the new copper evaluation will contribute to the overall improvement of nuclear data. Due to the interdependent nature of nuclear data, mathematically described by the covariance, the reduction of the uncertainty in the evaluation of one isotope will allow for the reduction in the uncertainties of other isotopes. Currently, in the computational modeling of criticality safety systems the uncertainty on \(k_{eff}\) is inferred by the propagation of nuclear data uncertainties rather than the uncertainty of the numerical solvers (i.e. stochastic uncertainty on \(k_{eff}\) of MCNP simulations).
Therefore, reducing the uncertainty on the nuclear data is the primary mechanism for reducing the uncertainty on the computed $k_{eff}$.

In the safety-oriented nuclear engineering world, managing uncertainties on fundamental parameters is crucial. With so much concern placed on not ever having a criticality accident in fuel storage, processing and transportation, the designers of these systems must be absolutely certain that such an event can never occur. However, large uncertainties in the neutron cross sections of materials used in these systems, such as copper, propagate through the modeling process and result in large uncertainties in the predicted behavior of the system. When it comes to the question of the probability of nuclear criticality accidents, large uncertainties are simply unacceptable. Without reducing the uncertainties on the input neutron cross section for the structural materials by evaluating new experimental data, the only solution to the safety concern is to severely over design these systems. The practice of over designing these systems involves either putting less fuel in the storage containers than the calculated minimum or putting more neutron absorbing materials around the fuel in order to compensate for the fact that the behavior of these systems cannot be calculated from fundamental parameters to within a reasonable uncertainty. This practice is economically wasteful in two regards. First, there is obviously additional money spent on the materials and construction of a container or facility for a nominal amount of fuel material that has been designed larger than it needs to be. Second, in such a practice, the extra money spent does not go at all to mitigating the problem in the future. On the other hand, investing the funds in better the nuclear data; the fundamental input for the calculations and the source of most of the final uncertainty, does result in less uncertainty on the predicted behavior of these systems in the future. With new cross section evaluations and reduced uncertainties on the cross section, the uncertainty on the modeling of nuclear systems will continue to decrease until the nuclear data is no longer the major source of uncertainty is the predicted behavior.

The interconnectedness of nuclear data, described above, reveals another hidden economic benefit from a new neutron cross section evaluation of copper. Many of
the ICSBEP criticality safety benchmark experiments were proposed, designed and built with the primary goal of benchmarking neutron cross sections for a specific set of isotopes of interest. There are many other uses for those experiments as well, but their primary purpose was to allow the evaluations of important isotopes to be validated in an integral manner. For example, the Zeus, intermediate-spectrum experiments were designed to test the neutron cross section of $^{235}$U in the intermediate energy range as well as the cross sections of copper and graphite. However, at the current state of the evaluated data libraries, the Zeus critical benchmarks are of not much use in benchmarking the $^{235}$U intermediate energy neutron evaluation because of the large uncertainty in the final integral parameters that propagates from the uncertainty in the copper evaluation. A new resolved resonance region (RRR) evaluation for copper with reduced uncertainties will revive the Zeus criticality benchmark experiment to its original intent and purpose. This is an example of how, due to the interconnectedness of nuclear data, new copper cross section evaluations can influence the improvement of the $^{235}$U cross section.

The goal of this Ph.D. work was to produce new, more accurate resolved resonance region evaluations for the two isotopes of copper, $^{63,65}$Cu, by developing a systematic feedback loop between integral and differential experiments. Such a feedback loop has been applied to the preliminary evaluations to produce new $^{63,65}$Cu resonance evaluations superior in quality to those possible based on differential experimental data alone. Several new approaches to evaluating the differential experimental data were also implemented for the preliminary resonance evaluation. Experimental cross section measurements versus energy in the thermal energy region were conducted for the first time for the isotopes of copper. New experimental data in this energy region allowed for a unique and more accurate treatment of the negative energy external levels in the resonance evaluations. Furthermore, the capture cross section has been experimentally measured and evaluated for copper for the first time. The resolved resonance region of the two copper isotopes was extended three-fold, from 99.5 keV to 300 keV. Hundreds of new resonances have been identified for each isotope and an automated program has been developed to identify the quantum angular
momentum of each resonance. The state of the art Reduced R-matrix approximation of the Reich-Moore formalism has been used for the new evaluations. Along the way, studies of the statistical distributions laws of quantum physics were carried out in the context of the resonance region of copper. Differential scattering cross sections were generated and utilized for improving the performance of neutronics codes. A study of the impact of high fidelity angular distributions was made and the results point to a non-trivial effect on criticality as well as more self-consistent nuclear data. The mathematical formulation for the temperature broadening of angular distributions was also developed. Realistic uncertainty and covariance data was generated. All of the new methodology developed in this research, has been developed for general resolved resonance region evaluations and can be fully applied to elements other than copper. The new methods can be applied to new and existing evaluations to extend and improve the resolved resonance region evaluations, and consequently cross section data libraries, beyond the limitations of only evaluating differential experimental data.

1.1 Experimental Data

Experimental cross section data versus incident neutron energy, the basis for resolved resonance region evaluations, was quite limited for $^{63,65}\text{Cu}$ before this work. Only two sets of transmission data were previously measured for each isotope of copper. As will be discussed in Section 2.2 it is near impossible to produce a resolved resonance region evaluation for general use on such a limited amount of experimental data. The only other experimental data supporting a resonance evaluation of copper came from integral cross section measurement techniques, described in Section 2.2.1. Integral cross section measurements result in a single cross section value representing the reaction cross section over a set energy range, such as the thermal energy region. This data, while useful, is not an ideal experimental method for resolved resonance region analysis.

The two sets of transmission data that had been measured before the beginning of this work come from measurements made by Pandey, et al. at O dela [28] in 1977.
The first of these data sets is from 32 eV to 185 keV and the second data set is from 1 keV to 1.4 MeV. The first data set has better energy resolution than the second set in the energy region below 10 keV. The second data set has significantly better energy resolution at energies above approximately 60 keV.

To address this deficiency in the experimental cross section data, three new experimental measurements have been made during the course of this research. The total thermal cross section versus energy was measured for the two isotopes of copper for the first time at the MIT Nuclear Reactor (MITR-II) using the time-of-flight (TOF) technique. See Section 3.1 for a detailed description of the experiment and Section 4.1 for the results. This experimental data was important in the evaluation work since it adds vital information for deriving good resonance parameters and uncertainties in the thermal energy region which integral cross section measurements in the thermal energy region cannot do alone. In addition, the measured total cross section data in the thermal range is also useful since it adds in the determination of energy bound levels for the compound nucleus (negative energies), see Section 3.2.3. Also for the first time, the capture cross section has been measured for the two isotopes of copper (see Section 2.2.1). Experimental capture data is vital to completing a new resolved resonance region evaluation as will be fully discussed with examples in several of the subsections of Section 2.2.

1.2 Resolved Resonance Region Evaluation

The copper RRR evaluations in the ENDF/B-VII.1 library are based on the resonance parameters from Neutron Cross Sections, Vol I by Mughabghab [25]. The authors of the copper evaluations contained in the ENDF/B-VII.1 library used these resonance parameters to fit the transmission data of Pandey et al. [28]. The upper bound on the energy of the resolved resonance region evaluation in ENDF/B-VII.1 was chosen simply where the resonance parameters of Mughabghab [25] stopped fitting the experimental data. No effort was made to identify new resonances at higher energies, even though there was experimental data available. The authors of the
ENDF/B-VII.1 $^{63,65}$Cu evaluations noted that the fit to the experimental data was improved when an additional constant background was added. However, this yielded a total average cross section that was too large. In addition, the original authors indicated the need to include a capture background from 60 keV to 99.5 keV. It is noted here that the original evaluation for both isotopes did not include experimental capture data.

There are several statistical laws that any resolved resonance region evaluation can be tested against. The following three are the best known: 1) Wigner’s law for the average level spacing of resonances, 2) Porter-Thomas resonance width distribution law 3) the Dyson and Mehta Long-Range Correlation of $\Delta_3$ Statistics Test for the number of levels versus energy. The exact physics of all three of these laws are laid out in the SAMDIST: A Compture Code for Calculating Statistical Distributions for R-matrix Resonance Parameters manual [20] and summarized in the following.

1. Wigner’s law for the average level spacing of resonances: the difference in energy between two consecutive resonance energies, $D_i$, for the same total quantum angular momentum and parity exhibits random behavior. The statistical distribution that best describes this behavior is called Wigner’s law.

\[
p(x)dx = \frac{\pi x}{2} \exp\left(-\frac{\pi x^2}{4}\right) dx
\]

where $x = D_i < D >$ with $< D >$ being the average of $D_i$.

2. Porter-Thomas resonance width distribution law: the resonance widths, $\Gamma_\lambda$ for resonances of the same total quantum angular momentum and parity has experimentally been shown to follow a $\chi^2$ distribution. For one degree of freedom, this distribution is known as the Porter-Thomas resonance width distribution law.

\[
p(x)dx = \frac{1}{\sqrt{2\pi x}} \exp\left(-\frac{x^2}{2}\right) dx
\]

where $x = \Gamma_\lambda < \Gamma >$ with $< \Gamma >$ being the average of $\Gamma_\lambda$. 

31
3. Dyson and Mehta Long-Range Correlation of $\Delta_3$ Statistics Test for the number of levels versus energy: the Dyson and Mehta Long-Range Correlation states that the number of observed energy levels should fit a straight line with respect to energy within a certain mean-square value and associated uncertainty. The definition is,

$$\Delta_3 = \min_{(a,b)} \frac{1}{n} \int_{E_i}^{E_f} (N(E) - aE - b)^2 dE$$

(1.3)

where $n$ is the number of resonances between energies $E_i$ and $E_f$ and $N(E)$ is the cumulative number of energy levels. The test predicts that the average theoretical value of $\Delta_3$ with associated standard deviation is,

$$\Delta_3 = \frac{1}{\pi} (\ln(n) - 0.06871) \pm \frac{\sqrt{1.169}}{\pi^2}$$

(1.4)

It was found that the ENDF/B-VII.1 evaluation did not agree well with any of these statistical laws. For example, the average level spacing for different quantum angular momenta governed by Wigner's law is given in Table 1.1.

In the ENDF/B-VII.1 evaluation, the angular distribution of secondary neutrons for elastic scattering was originally generated with the GENOA code. The angular distributions are represented as coefficients of Legendre polynomials. The ENDF formalism for angular distributions will be shown in Section 2.2. There are only 4 energy points across the ENDF/B-VII.1 resolved resonance region for the representation of the angular distribution. They are 1e-5 eV, 0.0253 eV, 10 keV and 100 keV. With the new resolved resonance region extended to up to 300 keV, the fifth energy point at 300 keV is picked up. Obviously, this cannot be considered a high fidelity model.

<table>
<thead>
<tr>
<th>Angular Momentum</th>
<th>$^{63}$Cu</th>
<th>$^{65}$Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>s-wave</td>
<td>p-wave</td>
</tr>
<tr>
<td>Mughabghab [24]</td>
<td>722±47 eV</td>
<td>404±22 eV</td>
</tr>
<tr>
<td>ENDF/B-VII.1</td>
<td>523±53 eV</td>
<td>2268±775 eV</td>
</tr>
</tbody>
</table>

Table 1.1: Average level spacing for different angular momenta for $^{63}$Cu and $^{65}$Cu.
of angular distribution. It is noted in the ENDF file that angular distributions can be calculated by the user on a finer energy grid from the resonance parameters. This however, is not the option that is used.

Angular distributions of elastic scattering in the resolved resonance region on a sparse energy grid results in inconsistent nuclear data. Physically, the angular distribution of elastic scattering can be reconstructed from the resonance parameters and will have physical resonances at the resonance energies. Treating angular distributions on a sparse energy grid ignores the resonance behavior of the angular distributions and only gives an average behavior. Furthermore, not including resonances in the angular distribution, directly contradicts the instructions laid out in the ENDF manual, “Care must be exercised in selecting an incident energy mesh for certain light-to-medium mass materials. Here it is important to relate any known structure (resonances) in the elastic scattering cross section to the energy dependent variations in the angular distributions. These two features of the cross sections cannot be analyzed independently of one another. Remember, processing codes operate on MT=2 (elastic scattering) data that are given in Files 3 (cross sections) and 4 (angular distributions). (Structure of the total cross section is not considered when generating energy transfer arrays). It is better to maintain consistency in any structure effects between File 3 (cross sections) and File 4 (angular distributions) data than to introduce structure in one File and ignore it in the other.”. Also, temperature broadening of the angular distribution is not possible with an average treatment. The mathematical formulation of the temperature broadening of angular distributions is derived in Section 3.2.4.

In this work, a new resolved resonance region evaluation has been completed. A new routine has been developed for identifying the quantum angular momentum of resonances, external levels have been evaluated and special treatment, allowed by the newly measured experimental data, has been given to negative external levels. All of the methodology used in the new resolved resonance region evaluation is documented in Section 3.2. The quantum angular momentum distributions for the new evaluations have been generated, along with the angular distributions for the elastic scattering
cross section and the self-shielded cross section. All of these results are presented in Section 4.2.

1.3 Benchmarking

A survey of the possible benchmark experiments has revealed that there are many critical experiments documented in the ICSBEP containing copper. However, for many of these experiments, there are only trace amounts of copper in the materials or the copper is not in a neutronically-important location. Table 1.2 contains the list of criticality safety benchmarks where copper was identified to be important in criticality safety of the system. Appendix C contains more detailed information on each of the benchmarks selected. These are often scenarios where copper is considered the primary or secondary\(^1\) reflector material, neutron absorbing material or separation material. Other benchmark experiments were also considered if the isotopes of copper accounted for a large percentage of neutrons captured in the system.

In addition to benchmark experiments currently documented in the ICSBEP, there are three more groups of criticality safety benchmarks identified in the NCSP Five Year Plan [26] to be completed that contain significant amounts of copper. They are listed in Table 1.3 with a brief description of the set up.

The entire procedure used to benchmark the new resolved resonance region evaluations is outline in Section 3.3. The results of applying the benchmarking procedure are presented in Section 4.3.

1.4 Coupled Differential and Integral Data Analysis

Accurate evaluated nuclear cross section data are needed for transport calculations for nuclear applications. In the cross section evaluation procedure, data evaluators

\(^{1}\)As in the in the examples of alloyed materials such as Duralumin (Al, Fe, Cu) or Ni-Cu-Zn Alloys
Table 1.2: List of ICSBEP benchmarks used in benchmarking the new copper evaluation

<table>
<thead>
<tr>
<th>ICSBEP Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF072-01</td>
<td>Zeus: Fast-Spectrum Critical Assemblies with an Iron-HEU Core Surrounded by a Copper Reflector</td>
</tr>
<tr>
<td>HMI006-01</td>
<td>The Initial Set of Zeus Experiments: Intermediate-Spectrum</td>
</tr>
<tr>
<td>HMI006-02</td>
<td>Critical Assemblies With a Graphite-HEU Core Surrounded by a Copper Reflector</td>
</tr>
<tr>
<td>HMI006-03</td>
<td></td>
</tr>
<tr>
<td>HMI006-04</td>
<td></td>
</tr>
<tr>
<td>LCT009-10</td>
<td>Water-Moderated Rectangular Clusters of U(4.31)O₂ Fuel</td>
</tr>
<tr>
<td>LCT009-11</td>
<td>Rods (2.54-cm Pitch) Separated by Steel, Boral, Copper, Cadmium, Aluminum, or Zircaloy-4 Plates</td>
</tr>
<tr>
<td>LCT009-12</td>
<td></td>
</tr>
<tr>
<td>LCT009-13</td>
<td></td>
</tr>
<tr>
<td>LCT009-14</td>
<td></td>
</tr>
<tr>
<td>LCT009-15</td>
<td></td>
</tr>
<tr>
<td>LCT012-09</td>
<td>Water-Moderated Rectangular Clusters of U(2.35)O₂ Fuel</td>
</tr>
<tr>
<td>LCT012-10</td>
<td>Roads (1.684-cm Pitch) Separated by Steel, Boral, Boroflex, Cadmium, or Copper Plates (Gadolinium Water Impurity)</td>
</tr>
<tr>
<td>LCT013-06</td>
<td>Water-Moderated Rectangular Clusters of U(2.35)O₂ Fuel</td>
</tr>
<tr>
<td>LCT013-07</td>
<td>Roads (1.684-cm Pitch) Separated by Steel, Boral, Boroflex, Cadmium, or Copper Plates with Steel Reflective Walls</td>
</tr>
<tr>
<td>LCT016-15</td>
<td>Water-Moderated Rectangular Clusters of U(4.31)O₂ Fuel</td>
</tr>
<tr>
<td>LCT016-16</td>
<td>Roads (1.892-cm Pitch) Separated by Steel, Boral, Boroflex, Cadmium, or Copper Plates with Steel Reflective Walls</td>
</tr>
<tr>
<td>LCT016-17</td>
<td></td>
</tr>
<tr>
<td>LCT016-18</td>
<td></td>
</tr>
<tr>
<td>LCT016-19</td>
<td></td>
</tr>
<tr>
<td>LCT016-20</td>
<td></td>
</tr>
<tr>
<td>LCT042-06</td>
<td>Water-Moderated Rectangular Clusters of U(2.35)O₂ Fuel</td>
</tr>
<tr>
<td>LCT042-07</td>
<td>Rods (2.032-cm Pitch) Separated by Steel, Boral, Copper, Cadmium, Aluminum, or Zircaloy-4 Plates</td>
</tr>
</tbody>
</table>

Table 1.3: List of new ICSBEP benchmarks containing copper from the Five-Year Plan

<table>
<thead>
<tr>
<th>ICSBEP Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LEU-COMP-THERM-TBD</td>
<td>Two LEU fuel rod arrays separated by large absorbing screens (Fe, Ni, Zr, Al, Pb, Cu)</td>
</tr>
<tr>
<td>LEU-COMP-THERM-TBD</td>
<td>Four LEU fuel rod arrays separated by large absorbing screens (Fe, Ni, Zr, Al, Pb, Cu)</td>
</tr>
<tr>
<td>IEU-MET-FAST-022 (SWEDEN)</td>
<td>Diluted 20%-enriched “cylindrical” uranium metal reflected by copper.</td>
</tr>
</tbody>
</table>
include measured differential data from facilities such as ORELA with nuclear physics models in order to obtain the best representation of the measured data with covariance data. The evaluated differential data are tested and validated using radiation transport codes to compute measured integral parameters (i.e., neutron multiplication factor) in well-characterized benchmark experiments. Typically, the benchmark testing results are communicated to the nuclear data evaluator with limited or qualitative information that can be difficult to utilize in order to improve the differential evaluation.

The process of differential evaluation of the resolved resonance region is a mathematically over determined problem with no exact solution. Therefore, there is much choice left to the evaluator in seeking parameters that minimize a certain metric. Even once an evaluation is considered complete based on differential experimental data it is not unique and other possibilities exist that may satisfy the metrics used to determine the accuracy of the evaluation. A complete evaluation is not unique, simply because of the fact that the experimental data being analyzed has an associated uncertainty. Simply put, the experimentally measured cross section value at every energy point is only reported as a mean value and a standard deviation. Therefore, it is statistically equivalent for the reconstructed cross section (from the resonance parameters) to pass above or below the mean experimental value by the same amount. This ambiguous choice has been previously left simply to the expertise of the evaluator.

Much of the systematic uncertainty on differential cross section data comes from the normalization of capture and inelastic cross section measurements. These measurements rely on the experimenter having a high degree of knowledge of the experimental flux. Unfortunately, this is not always the case. In the best case, this results in larger uncertainties over certain energy regions of the experimental data. In the worst case, the experimental cross section data is miss-reported whether it is in the way of systematically larger or smaller mean values for the measured cross section or small uncertainty that does not reflect the actual state of knowledge. Unlike, the case of statistical uncertainty, systematic uncertainty can result in resolved resonance evaluations that produce a cross section that is too high over a large energy region.
It is, therefore, the uncertainty on the normalization of experimental data, which is of biggest concern in completing a new resolved resonance region evaluation based on differential experimental data.

Providing additional information that may dissolve ambiguity between equivalent choices can help this problem. In the case of differential cross section evaluation, the additional helpful information comes from integral experiments. Valuable information can be extracted from well-known integral experiments and used as a guide in the differential analysis. If the choice of having the cross section pass above rather than below an experimental point by the same amount (or visa-versa) results in an overall better performance in integral benchmark calculations, it must be the correct choice in the previously ambiguous decision. The TSURFER module of the Standardized Computer Analyses for Licensing Applications (SCALE) [4] code package is a tool capable of suggesting multi-group data adjustments based on nuclear data performance in integral benchmark calculations. The methodology of the TSURFER code is briefly described in Section 2.4 and fully in the SCALE6 manual [4].

However, the TSURFER code only provides multi-group cross section adjustments which does not adjust the neutron cross sections in a self-consistent method nor take into account any information from experimental cross section measurements. The current implementation of TSURFER cannot provide suggested changes for differential cross section with respect to angle (sometimes referred to as, 2-Dimensional cross section data) nor double differential cross sections with respect to angle and outgoing energy (sometimes referred to as 3-Dimensional cross section data). Adjusting the integrated cross section, without adjusting the underlying differential cross section results in self-inconsistent nuclear data. Furthermore, multi-group cross section adjustments done with the TSURFER code do not take into account either the experimentally measured cross sections nor the reported uncertainty of those experimental measurements. Therefore, it is possible for TSURFER to suggest cross section changes that will be inconsistent with experimental cross section measurements.²

²Much care must be given to generate proper covariance matrices for the resonance parameters and the individual reaction cross sections in order to prevent this from happening. High fidelity covariance analysis is rare in nuclear data.
In the methodology developed as part of this research, the multi-group cross section adjustments suggested by TSURFER are coupled directly to changes in the resonance parameters of the resolved resonance region. Cross section values, reconstructed from resonance parameters, are only changed within the uncertainty of the experimental data. By coupling the suggested data changes from integral experiments directly to the resonance parameters, the double differential cross sections are adjusted simultaneously and consistently with the angle-integrated cross sections. Furthermore, the covariance data of the resolved resonance region evaluation is updated to reflect the true state of knowledge. Previous to this work, no methodology existed for using information from integral benchmarks to update the evaluation of the covariance data.

The overall objective of this project was to couple, for the first time, the modern R-matrix resonance analysis tool SAMMY [17] with modern radiation transport sensitivity/uncertainty (S/U) analysis tools to enable differential cross section evaluations to be developed with the pertinent integral data. Such a tool ties together the basic science research tool with the nuclear application analysis tool thereby enabling the streamlined analysis of measured cross section data to produce cross section evaluations with covariance data for use in radiation transport analyses of nuclear systems. In this work, the analysis tool has been developed and used to analyze recently obtained data for both copper isotopes to produce new cross section data libraries that have been demonstrated in criticality safety application analysis.
Chapter 2

Background

2.1 Introduction to Nuclear Data

Nuclear data is used in almost all aspects of the nuclear science and engineering industry. Microscopic cross sections, which can be simply defined as a measure of the probability of interaction between neutrons of different energies and the nucleus, make up a vast portion of the nuclear data field. The microscopic cross section of all isotopes have several distinct regions that appear with increasing energy of the incident neutrons. Figure 2-1 gives the names and order of the different neutron energy regimes that appear in all microscopic cross sections. The microscopic cross sections behave differently in different energy regimes.

- Thermal Energy Region: This energy region is defined up to the energy of the first nuclear resonance that appears in a given isotope. The energy of the first resonance for a given isotope is determined by the nuclear structure of that isotope, but typically occurs somewhere between 1 eV and 1 keV. In the thermal energy region, the behavior of the cross section is smooth, with the capture reaction cross section roughly behaving\(^1\) as \(1/\sqrt{E}\) and the scattering cross section being roughly constant and governed by potential scattering.

\(^1\)Section 2.2 discusses the fact that the \(1/\sqrt{E}\) behavior is an approximation rather than an exact phenomenon
• Resolved Resonance Region: Nuclear resonances at neutron energies determined by the structure of the nucleus introduce extreme fluctuations in the neutron cross section. The neutron is much more likely to interact with the target nucleus when the energy of the incident neutron falls at one of the excited states of the compound nucleus. The compound nucleus is the name of the short lived state that the target nucleus and the incident neutron form immediately after contact. The resolution of experimental machines is smaller than the width of the resonances in this energy region. Therefore, resonances can be distinguished or seen individually rather than just the lump behavior being measured. Cross section representation of the thermal and the resolved resonance region can be made by resonance parameters. The details of the quantum mechanical models describing these regions are given in Section 2.2

• Unresolved Resonance Region: Even though, the physics of the nuclear interaction does not change in the transition from the resolved resonance region to the unresolved resonance region, the capability of the experimental machines changes. The experimental resolution goes from being smaller than the width of the resonances to being larger than the width of the resonances. Individual resonances can no longer be recognized. In practice, another consideration can come into play in determining where the resolved resonance region stop and the unresolved begins. Often the unresolved resonance region begin where the resonance self-shielding of the isotope’s cross section no longer matter even though the resolution of the differential experimental measurements can stretch far beyond this energy. The amount of effort involved in doing a resolved resonance region evaluation outweighs the benefits to reactor physics of the improved state of knowledge of the cross sections. The cross sections in the unresolved resonance region are represented in the form of probability tables. For most isotopes the unresolved resonance region lies somewhere between 1 keV and 1 MeV. However, unresolved resonance region evaluations do not exist for all isotopes that have resolved resonance region evaluations.
- High Energy Region: Above the upper limit of the resolved or unresolved resonance region evaluation (if one exists) the bulk behavior of the cross section is best described by the parameters of an optical model of the nucleus. The most widely used model in the nuclear industry the Hauser-Feshbach model. The reconstructed cross section models the bulk behavior of the cross section with smooth wide oscillations spanning the energy region typically from above 1 MeV up to 20 or 200 MeV.

In general microscopic cross sections can be said to be a combination of raw experimental data and quantum mechanical models of the nucleus. A simplified schematic of the life cycle of nuclear data is provided in Figure 2-2. In general, everything begins with the experimental measurement of the reaction cross sections versus the incident neutron energy (differential cross section measurements). The measurements are made to a predetermined required quality based on the sensitivity and uncertainty analysis of earlier cross section data performance in sample calculation problems. Next, in what is known as the evaluation process, quantum mechanical models of the nucleus are used to fit continuous curves through the numerous experimental data points for different reaction types. From this stage, the evaluator and the experimentalist may go back and forth, with the evaluator requesting more or different experimental data based on how well the model parameters fit the available experimental data. Then, the parameters of the quantum mechanical model calculated in the evaluation process are used to reconstruct the cross sections via cross section processing codes. The processing codes deliver either continuous energy cross sections or multi-group cross sections that are processed into forms usable by neutron transport codes. Recognizing that neither the experiments nor the quantum mechanical models are perfect, benchmarking of integral experiments is done using the evaluated data. The results of the benchmarking process give the evaluator non-quantitative feedback on the status of the evaluation. The new evaluation may have performed better on some integral benchmarks and worse on others. It is up to the evaluator to decipher what to change in the new evaluation based on the benchmark results. No systematic feedback loop exists between the evaluation process and the
Figure 2-1: A diagram showing the different regions of microscopic cross sections. The fictitious line in the graph gives an illustration of the behavior of the cross section in each energy region.
benchmarking on integral experiments. The evaluation is then adjusted to the best judgment and experience of the evaluator, sometimes through many iterations, to be in better agreement with integral experiments. Sensitivity analysis of the benchmark experiment models to the input cross sections is sometimes done. The result of the uncertainty analysis has been used to determine the level of uncertainty that needs to be requested of the experimental data such that a smaller amount of uncertainty will propagate down the entire process and result in smaller uncertainty on the integral benchmark calculations. Recently, a feedback loop has been proposed for adjusting the input multi-group cross sections based on the sensitivity analysis of benchmark models with multi-group cross section inputs. A more detailed overview of this technique is given in Section 2.4. Once the evaluator is satisfied with the fit of the differential experimental data and the evaluation is shown to perform well on relevant integral experiments, the data is released to general purpose libraries available to the end user.

Differential experimental measurements produce cross section values versus incident neutron energy, then the experimental data is reduced to a base set of model parameters and then the cross section is reconstructed and formatted to be used in neutron transport codes. Seemingly, the evaluation process could just be eliminated and cross section values, direct from measurement, could be used in transport calculations. However, this is not the case. To begin with, while differential cross section measurements attempt to measure the true neutron cross section, what is actually recorded is the convolution of the true neutron cross section and a whole set of experimental complications such as resolution function and many more listed in Section 2.2. Using these values would not reflect reality. Furthermore, model parameters allow the cross section to be reconstructed under any conditions. For example, the cross section can be reconstructed to any temperature using Doppler broadening. Finally, the model parameters allow the nuclear data to be stored compactly. Experimental data of several different reaction types, even similar experiments with different measured values and uncertainties as well as measured angular distributions can go into the same set of model parameters. Using the model parameters allows the evaluat-
tor to encompass all of the experimental data, find compromises between conflicting experimental results and combine complimentary data in a compact way. Later, the model parameters can be used with the same physical model to reconstruct the cross section for the same or different reaction type than those measured.

2.2 Resolved Resonance Region Evaluation

Figure 2-2 has given an overarching introduction to the life cycle of nuclear data. In this Section, the individual pieces of the life cycle of nuclear data will be examined in greater detail and from a practical perspective. An overview of some of the experiments used to measure cross sections will be given. The quantum physics model of nuclear cross sections will be discussed as well as the practical approximation of the full model and its implementation in the computer code SAMMY will be given. The definition of the differential elastic scattering cross section with respect to angle is given to aid in further discussion of the importance of angular distributions in criticality safety as well as the derivation of the mathematical formulation for temperature broadening of angular distributions. Next, the processing codes that reconstruct the cross sections from the model parameters will be reviewed. Finally, the codes of the sensitivity and uncertainty analysis of integral experiments, TSUNAMI and TSURFER of the SCALE code package, will be described as well as the current practices of the feedback that these codes are used to provide. The work carried out for this research project will serve as a backdrop for all of the following discussions.

2.2.1 Experimental Measurements

Before this work, there were no experimental measurements for the thermal cross section of the two copper isotopes, $^{63,65}\text{Cu}$, available in the EXFOR [32] data base. Several measurements are available of the thermal value of the total and radiative capture cross sections for both isotopes using integral measurement techniques. The total cross section in the integral technique is measured using a well characterized thermal flux profile. A sample of known size, density and isotopic composition is
Figure 2-2: A flow chart showing the life cycle of nuclear data.
placed in a neutron field. A simple measurement of the reduction of the neutron flux, tells the experimenters the neutron transmission value of the sample. Knowing the flux profile and assuming a $1/v$ cross section shape, one can easily calculate the thermal cross section. The thermal cross section is then reported as a single value at the thermal neutron energy of 0.0253 eV. The thermal capture cross section is measured in a similar but more complex way. A well characterized thermal neutron flux is used once again. A sample of known properties is then placed in the neutron field and left for a recorded period of time. During the time of the irradiation, the sample undergoes $(n, \gamma)$ reactions among many others. This $(n, \gamma)$ reaction results in the production of a new isotope with one more neutron than the target. For the technique of activation analysis measurement of the thermal capture cross section it is usually a requirement that this new isotope be unstable and decay with a convenient half life. Convenient simply refers to the fact that the half life be in the range where further measurement of the characteristic gamma rays from the decay of this isotope be experimentally feasible. The characteristic gamma ray spectrum of the activated sample is then recorded. The counts are corrected for any gamma ray geometric self-shielding in the sample, and the total number of activated isotopes is deduced at the time of the irradiation taking into account the decay rate. From this, once again, knowing the flux characteristics and taking the $1/v$ approximation, the experimenters are able to deduce the thermal capture cross section. Once again, the cross section is reported as a single value at the thermal neutron energy. The total and capture thermal cross section values of both isotopes are quoted in the Atlas of Neutron Resonances, [24].

While integral cross section measurements are certainly helpful in doing resolved resonance region evaluation in the absence of other experimental data in the thermal energy region, there are several problems with using such data. First of, these measurements are deduced from integral measurements, resulting in a single cross section value at the thermal energy value of 0.0253 eV. Therefore, this data cannot be used to fit a cross section versus energy in the thermal energy region. The assumption that is usually made that the shape of the cross section in the low energy range follows a $1/v$
shape is taken to be law and carries no uncertainty with it. However, as described by Wigner in his 1948 original paper, the radiative capture cross section is only $1/v$ in the first order approximation and is dependent on $v$ in the next order term. Therefore, simply assuming the $1/v$ dependence may be inaccurate for some isotopes. Integral cross section measurements, with no energy discrimination systems allow for very large count rates and therefore result in small Poisson statistics. It has been the usual practice in the world of neutron cross section evaluations to extend the uncertainty on the single datum point measured by the integral technique to the fitted cross section in the entire thermal region. Extending the uncertainty of a measured datum point at one energy value across the entire region is not justified. Therefore, cross section measurements with neutron energy discrimination in the thermal energy region are necessary for a good evaluation. Such measurements, reveal the value of the thermal cross section, the true shape of the cross section in the thermal energy region and reflect the true state-of-knowledge behavior of the uncertainty across the thermal energy region. Furthermore, shape of the cross section in the thermal energy region influences the choice of the negative energy external resonance parameters as will be discussed in Section 3.2.3.

There were no experimental measurements of the copper capture cross section in the resolved resonance region made before the beginning of this work. Two sets of the capture cross section measurements were made for this effort by Klaus Guber, et al. [13] at the GELINA experimental facility in Geel, Belgium in 2011. The first of these measurements runs from 100 eV up to 90 keV and the second from 100 eV up to 300 keV. A summary of all the experimental data used for the resolved resonance region evaluation carried out in this work is given in Table 2.1.

The capture cross section measurements performed at GELINA were done using the time-of-flight technique to obtain the neutron energy. The experimental principle was in fact very similar to that used in the original experiments to attempt to measure the capture cross section in the thermal energy range during this research. The principle of that experiment is fully described in Appendix B and is therefore not repeated here. Unlike, the MIT capture experiment described in Appendix B, the
capture measurements made at GELINA were normalized using the characterization of the experimental flux. This is currently standard practice for capture and inelastic cross section measurements. As has been discussed in Section 1.4 such practice has the danger of introducing systematic uncertainties into the experimental data and the evaluator has to trust the experimentalist that the reported uncertainties are correct and true. For this research, the newly developed differential-integral coupling methodology, introduced in Section 1.4 and detailed in Section 3.4, was used to alleviate this issue.

Experimental capture data is vitally important to the evaluation process. Capture experiments reveal resonances that are not seen in transmission experiments. It is also possible to approximate the quantum angular momentum of a resonance from the integral of the capture resonance. Finally, capture experimental data provides an inside look at what the cross section looks like inside black resonances\(^2\) seen in the transmission experimental measurements. Examples are provided in Figure 2-3 and Figure 2-4. Unlike Figure 2-3, the black resonance in the total cross section of Figure 2-4 is hiding two resonances that would not have been identified were it not for the capture data.

### 2.2.2 Overview of R-Matrix Theory of Nuclear Reactions

The R-matrix theory of nuclear reactions is the name of the physical model and the foundation of the evaluation of the resolved resonance region. The final form of the equations of R-matrix theory can be derived all the way from the Schrödinger

\(^2\)The term black resonance refers to a strong resonance in the total cross section. There is generally very poor statistics in the transmission experimental data around the peak of these resonances

<table>
<thead>
<tr>
<th>Reference</th>
<th>Energy (eV)</th>
<th>Facility</th>
<th>Measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pandey et al. [28]</td>
<td>32-185,000</td>
<td>ORELA</td>
<td>Transmission at 78 m</td>
</tr>
<tr>
<td>Pandey et al. [28]</td>
<td>1,000-1,400,000</td>
<td>ORELA</td>
<td>Transmission at 78 m</td>
</tr>
<tr>
<td>Guber et al. [13]</td>
<td>100-90,000</td>
<td>GELINA</td>
<td>Capture at 58 m</td>
</tr>
<tr>
<td>Guber et al. [13]</td>
<td>100-300,000</td>
<td>GELINA</td>
<td>Capture at 58 m</td>
</tr>
<tr>
<td>Sobes et al.</td>
<td>0.01-0.1</td>
<td>MITR</td>
<td>Transmission at 1.2 m</td>
</tr>
</tbody>
</table>
Figure 2-3: An example of a black resonance in the total cross section (bottom) for $^{63}\text{Cu}$ and the complimentary capture data (top). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty.
Figure 2-4: An example of a black resonance in the total cross section (bottom) for $^{63}$Cu and the complimentary capture data (top). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty. Unlike Figure 2-3, the black resonance in the total cross section is hiding two resonances that would not have been identified were it not for the capture data.
equation; the foundation of quantum mechanics. Very few assumptions have to be made along the way, and the final form of the full R-matrix equations are considered to have no significant approximations. The derivation of the final form from the Schrödinger equation is quite lengthy and requires significant knowledge of quantum mechanics and control of mathematical manipulations. Most of all, the derivation is presented and described in simple terms and excruciating details in many common references. Therefore, the final form of R-matrix theory is presented here and the interested reader is referred to the review article by Lane and Thomas [16] as the primary source and to the book by Foderaro [6], and two publications by Fröhner [8] [9] as supplementary materials.

To begin talking about the formulation of R-matrix theory, the term *channel* must be defined. A *channel* is defined as a pair of particles (incoming or outgoing) along with the associated information that describes the particles. Each *channel* can be described by the information that describes the individual particles involved, \( \alpha \), such as their mass, \( m \), charge, quantum spin, and parity as well as information describing the interaction of the two particles, such as the total quantum angular momentum, \( J \) and spin. For the analysis carried out in this research on resolved resonance region interactions of neutrons, only non-Coulomb channels were considered. This simplifies the R-matrix formulation.

Based on such definition of a *channel*, the angle-integrated cross section for a reaction from non-Coulomb entrance channel, \( c \), to non-Coulomb exit channel, \( c' \), with total quantum angular momentum, \( J \), is,

\[
\sigma_{cc'} = \frac{\pi}{k_\alpha^2} g_{\alpha} |\delta_{cc'} - U_{cc'}|^2 \delta_{JJ'}
\]  

(2.1)

This is the most general statement of the R-matrix formalism for neutron reactions. All of the individual pieces are described here after.

\( k_\alpha \) is the quantum wave number associated with the incident particle pair, \( \alpha \), \( g_{\alpha} \) is the statistical spin factor defined as,
\[ g_{Ja} = \frac{2J + 1}{(2i + 1)(2I + 1)} \]  

(2.2)

where \( i \) and \( I \) refer to the spin of the incident and target particles.

\( U_{ce'} \) is termed the scattering matrix (or sometimes the collision matrix) and further defined as

\[ U_{ce'} = e^{-i\phi} W_{ce'} e^{-i\phi'} \]  

(2.3)

where \( \phi \) is the potential scattering phase shift that will be defined recursively with respect to variables that will appear later on in this definition of the R-matrix model. The \( W \) matrix carries no well known name and is only defined as,

\[ W = P^{1/2} (I - R(S - B + iP))^{-1} (I - R(S - B + iP^*) P^{-1/2} \]  

(2.4)

where, \( P \) and \( S \) are the penetration factor and the shift factor respectively. The variable \( R \) represents the actual R-matrix which lends its name to the entire model. The identity matrix is \( I \) and \( B \) is a boundary constant chosen to be equal to the negative of the orbital angular momentum. The variables, \( P, S, \) and \( \phi \) are all recursive functions defined for each value of the orbital angular momentum. The definitions are based on a function, \( \rho \), which is the quantum wave number multiplied by a constant called the channel radius, \( a_c \). The channel radius, most basically put, is the interaction radius for the two particles. The recursive definition of \( P, S \), and \( \phi \) are,

\[ P_l = \frac{\rho^2 P_{l-1}}{(l - S_{l-1})^2 + P_{l-1}^2} , \quad P_0 = \rho \]  

(2.5)

\[ S_l = \frac{\rho^2 (1 - S_{l-1})}{(l - S_{l-1})^2 + P_{l-1}^2} - l , \quad S_0 = 0 \]  

(2.6)

\[ \phi_l = \phi_{l-1} - \tan^{-1} \left( \frac{P_{l-1}}{l - S_{l-1}} \right) , \quad \phi_0 = \rho \]  

(2.7)

At last, the actual R-matrix is defined as,
\[ R_{c'c} = \sum_{\lambda} \frac{\gamma_{\lambda} \gamma_{\lambda'} \delta_{jj'}}{E_\lambda - E} \]  \hspace{1cm} (2.8)

with, \( \lambda \) referring to a particular resonance, and \( E_\lambda \) and \( \gamma_\lambda \), the resonance energy and reduced width amplitude respectively, being the fundamental parameters of the model. This matrix carries the name of the entire formalism because it is the central piece. The actual R-matrix is the source of all of the interference effects observed in cross section. Interference effects are, in a way, non-linearities in the problem. For example, changing the resonance parameters of one resonance will affect the shape of the reconstructed cross section not only in the immediate neighborhood of that resonance but may also affect the shape of the cross section near another resonance, one that is far away in energy from the first one. There are also several different types of interference effect. The simple example described above, is known as level-level interference, where level refers to a resonance. This type of interference is hard to see mathematically immediately from this formulation of the R-matrix. Channel-channel interference, a different type of interference, is much easier to recognize from the R-matrix. The terms \( \gamma_c \) and \( \gamma_{c'} \) both appear in the numerator of the summation inside the R-matrix for the same resonance, \( \lambda \).

The R-matrix equation closes the full definition of the cross section for a reaction from entrance channel, \( c \), to exit channel, \( c' \). All of the terms above have been described in terms of the most fundamental quantities or parameters of the model. The fundamental model parameters of \( E_\lambda \) and \( \gamma_\lambda \) can only be determined through the optimization of the fit of the model to experimental data. Determining these parameters are the ultimate goal of a resolved resonance region evaluation.

2.2.3 SAMMY Code System for Resolved Resonance Region Evaluations

SAMMY is a widely used computer code for the parametrization and understanding of differential neutron induced cross section data based on the R-matrix formalism. SAMMY was originally developed by Oak Ridge National Laboratories (ORNL) to
analyze data from the Oak Ridge Electron Linear Accelerator (ORELA) but is now used throughout the world to analyze data from numerous accelerator facilities.

The R-matrix, as stated in the previous subsection, requires the summation of an infinite amount of channels. The number of open gamma ray channels is essentially infinite. This fact motivates the Reduced R-matrix formalism of Reich-Moore. The Reich-Moore approximation treats all of the gamma ray channels as aggregate with a single reduced width amplitude parameter. The reduced R-matrix form is,

$$R_{cc} = \sum_{\lambda} \frac{\gamma_{\lambda c} \Gamma_{\lambda c}^c}{E_{\lambda} - E - i\Gamma_{\lambda \gamma}/2} \delta_{jj'}$$  \hspace{1cm} (2.9)

where, the summation is now over particle channels only, not gamma channels. The variable $\Gamma_{\lambda \gamma}$ is used to indicate special treatment of the gamma channels and is strictly equal to $2\gamma_{\lambda \gamma}^2$. The code SAMMY uses this form of the R-matrix with the rest of the formalism as described above to find the optimum resonance parameters, $E_\lambda$, $\Gamma_{\lambda \gamma}$, and $\gamma_{\lambda c}$ base on the fit of the experimental data.

In the process of evaluating differential experimental data multiple sets of experimental data must be evaluated. The system used for the evaluation must be able to handle different sets of experimental data for the same reaction type, for different reaction types, for different measurement quantities (such as, differential cross section with respect to angle, $\delta \sigma/\delta \Omega$), and even for different isotopes. The evaluation code must be able to include all this experimental data in a systematic way. Importance of analyzing several data was already discussed at the beginning of this Section with the example of the importance of analyzing both the transmission and the capture data. Here, a different example is provided of the importance of including sample impurities in the analysis. Figure 2-5 shows an example of how valuable it is to include the impurities in the analysis. Both samples used in the capture experiments for $^{63}\text{Cu}$ and $^{65}\text{Cu}$ were more than 99% pure. However, the resonances of the other isotope can be seen in the experimental data of $^{65}\text{Cu}$. Without simultaneous analysis, proper treatment of the model parameters is impossible.

The SAMMY code uses Bayesian updating to update the model parameters as it
Figure 2-5: Plots of the experimental capture data of $^{63}$Cu (top) and $^{65}$Cu (bottom). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty. Even though the $^{65}$Cu sample is more than 99% pure, the resonance from the $^{63}$Cu impurity can be seen.
looks at several sets of experimental data. The basic statement of Bayes’ theorem is given below along with a description of how the individual pieces of the theorem are interpreted for the case of obtaining resonance parameters from experimental data based on the Reich-Moore formalism.

\[ p(P|DX) = p(P|X) \cdot p(D|PX) \]  \hspace{1cm} (2.10)

- \( P \) are the model parameters (resonance parameters) of the reduced R-matrix theory.
- \( D \) is the experimental data set being currently analyzed.
- \( X \) is the set of all experimental data previously analyzed to obtain the current set of model parameters.
- \( p(P|DX) \) is the joint probability density function for the model parameters updated based on the inclusion of the new experimental data. The covariance matrix associated with the joint probability density function provides a systematic evaluation of the certainty with which the model parameters can be determined as well as all of the interdependences between the model parameters. The first moment of the probability density function is the value taken for the final resonance parameter.
- \( p(P|X) \) is the joint probability density function of the model parameters before the current experimental data set was included.
- \( p(D|PX) \) is the joint probability density function of observing experimental data \( D \) given that the model parameters based on all previously considered experimental data, \( X \), are correct.

Using Bayes’ theory, SAMMY is able to analyze one set of experimental data (treating it as \( D \)), update the resonance parameters based on that experimental data (\( p(P|DX) \)), and from thereon, treat that set of experimental data as a part of the previously analyzed data (\( X \)). This way, each new set of experimental data is
analyzed with respect to the current resonance parameters and with the backdrop of all of the experimental data analyzed before. Afterwards, the experimental data set is retired into the prior. In this way, the resonance parameters of the reduced R-matrix theory are updated systematically and respecting all covariance data based on many experimental data sets.

Under the assumption of all of the probability density functions being normal, the prior distribution, can be written as,

$$p(P|X) \propto \exp\left(-\frac{1}{2}(P - \overline{P})'M^{-1}(P - \overline{P})\right)$$  \hspace{1cm} (2.11)

where, $\overline{P}$ is the exception value of the joint normal probability density function and $M$ the associated covariance matrix. The joint probability density function of observing the current experimental data assuming the current model parameters are correct, can be written as,

$$p(D|PX) \sim \exp\left(-\frac{1}{2}(D - T)'V^{-1}(D - T)\right)$$  \hspace{1cm} (2.12)

where now, $T$, is the cross section reconstructed for the current resonance parameters using the Reich-Moore formalism rather than being the expectation values of the experimental data. The matrix $V$ is the covariance matrix that takes into account both the reported uncertainty on the experimental data as well as any covariance that arise from reconstructing experimental data. All of the uncertainties on the parameters of the experimental set up, such as an uncertainty on the flight path for a time of flight experiment, enter this covariance matrix. A list of additional experimental considerations that will enter the data covariance matrix is given in Section 3.2.

In light of the Bayesian update method, the overall goal of the SAMMY analysis is to reduce the least-square $\chi^2$ test statistic between the experimental data and the expectation value of the reconstructed cross section.

$$\chi^2 = (D - \overline{T})'V^{-1}(D - \overline{T})$$  \hspace{1cm} (2.13)
where the difference between Eqn. 2.13 and Eqn. 2.12 is that $\overline{T}$ is the mean of the probability density function $T$. An intuitive way to interpret the $\chi^2$ value is to state that the goal of the resolved resonance region analysis is to derive the parameters such that the difference between the reconstructed cross section will have very little difference with any newly obtained experimental data $(D - T \rightarrow 0)$. In other words, the final resonance parameters should be able to predict the cross section for any reaction.

2.2.4 Definition and Differential Cross Section with Respect to Angle

The physically intuitive definition the differential scattering cross section with respect to angle is the probability that a neutron at a given incident energy scatters into solid angle $d\Omega$. The differential scattering cross section, $d\sigma_s(E)/d\Omega$ or equivalently written as $\sigma_s(E, \mu)$, can be calculated directly from the resonance parameters as a summation of weighted Legendre Polynomials. The exact weighting factors have a long and messy representation in terms of the resonance parameters and the quantum angular momentum of the resonances. These will not be presented here as their formulation has no influence on the discussions related to this work. The interested reader is referred to Blatt and Biedenharn [3] for the full formalism. More relevant, is the ENDF/B representation of the angular distributions of the scattering. The ENDF/B preferred method for representing and storing angular distributions are the coefficients of Legendre Polynomials. The definition of the coefficients, $\alpha_l$ is,

$$\alpha_l(E) = \frac{2\pi}{\sigma_s(E)} \int_{-1}^{+1} \sigma_s(E, \mu)P_l(\mu)d\mu \quad (2.14)$$

where, $\sigma_s(E)$ is the angle integrated scattering cross section.

Similar to $\sigma_s(E, \mu)$ and $\sigma_s(E)$ the angular distribution will naturally have fluctuations at the resonance energies and will be subject to temperature broadening. Examples of what the angular distribution looks like for $^{63,65}$Cu as a function of incident neutron energy will be given in Section 3.2.4.
The scattering angular distribution is traditionally an area that has received very little attention in nuclear data. Usually, the resolved resonance region evaluation is done based on evaluating experimental transmission and capture data. The angle integrated scattering cross section is then reconstructed from the optimum resonance parameters. However, the angular distribution for the scattering cross section is usually done by a different evaluator, using a different code and most often based on model calculations that result average angular distributions. Such is the case presented in Section 1.2 for the two isotopes of copper. This creates the problem, as noted in the quotation from the ENDF manual in Section 1.2, that the angular distributions are then inconsistent with the angle integrated cross section.

Evaluating the angular distribution of scattering is in a way the final frontier of resolved resonance region. One of the forms of the generic equation for criticality of a system can be written as,

\[
k = \frac{\int \nu \Sigma_f \varphi \, d\Omega}{\int (-\nabla \cdot D \nabla \varphi) \, d\Omega + \int \Sigma_a \varphi \, d\Omega} \tag{2.15}
\]

where, \(\Omega\) represents the entire phase space of the problem, \(\nu\) is the average number of neutrons per fission, \(\Sigma_f\) and \(\Sigma_a\) are the macroscopic fission and absorption cross section respectively, \(\varphi\), is the neutron flux, and the term \(-\nabla D \nabla \varphi\) can be interpreted as the leakage term. The leakage term, in general, accounts for the number of neutrons that leave the system by scattering out. More directly, the leakage term encompasses the differential scattering cross section with respect to angle. The term, final frontier, was used to reflect the fact that resolved resonance region evaluation pays close attention to the fission and absorption angle integrated cross sections, and until recently, has not payed much attention to the angular distribution data. As can be seen from the equation above, the term encompassing the angular distribution data plays as much a role in the criticality of a system, as do the other two. Consider the following physical example. Simple nuclear engineering suggests that a reflected nuclear reactor core has better neutron economy than a bare core. Effectively, one can make

\footnote{For non-fissile isotopes. For fissile isotopes, the resolved resonance region evaluation is traditionally done based on experimental transmission, capture and fission data.}
a smaller, more cost effective reflected nuclear reactor than just a bare core. From a design point of view, neutrons leaving the core and entering the reflector region should scatter back into the core for a more effective reactor. However, whether the neutrons undergo forward peaked scattering or backward peaked scattering depends on the angular distribution of scattering. Therefore, the angular distribution of scattering plays an important role in the criticality of the system. Further, a different example can illustrate the importance of angular distribution data to the criticality safety community. As discussed in Section 1, nuclear criticality storage and transportation canisters are designed in such a way that a criticality accident cannot occur. Here, similar to the reactor reflector, it is important to know the angular distribution of scattering, but in contrast to a reactor reflector, it is important for the materials to be forward scatters, so that neutrons will leak out of the system.

It is quite natural for scattering angular distributions to be reconstructed from resonance parameters for several reasons. The first reason being the desired consistency between angular and angle integrated data in ENDF evaluations. Second, it is a natural choice to reconstruct the angular distribution from the resonance parameters because in searching for the optimum resonance parameters by fitting the differential experimental data, the evaluator can be thought of as not determining the resonance parameters that will reproduce the experimental data, but rather trying to determine the actual physical model of the nucleus. Therefore, if the model using the resonance parameters represents the nucleus well, it must produce a consistent angular distribution. The assumption that the resonance parameters represent the physical nucleus well is key to this assertion, particularly, the quantum angular momentum of each resonance being assigned correctly. As discussed above, experimental data of the capture cross section is a huge asset in terms of determining the quantum angular moment of each resonance.
2.3 Processing Codes NJOY and AMPX

Processing codes give the user numerous options of how to reconstruct and format the cross section libraries from the final resonance parameters. The use of the processing codes is specific to a particular application or isotope. Therefore, the specific use of the processing codes with regards to this research and the two isotopes of copper shall be described below.

In this research the new evaluations were processed by two individual processing codes, NJOY and AMPX to make continuous energy and multi-group cross sections respectively. While performing similar tasks, the NJOY and AMPX code systems have completely independent capabilities. NJOY99.0 is a code system for producing pointwise and multi-group neutron and photon cross sections from ENDF/B data. [21] In the NJOY code system the resolved resonance parameter data was used to reconstruct point-wise cross sections. These cross sections were Doppler-broadened based on the kernel broadening method by integrating the integral equation defining the effective cross section. The AMPX [12] code system was used to perform the same task as NJOY but to create multi-group SCALE Master Libraries. In the AMPX code, a similar treatment of the resolved resonance region was applied, with the reconstruction of continuous energy cross section and then Doppler-broadening based on numerical integration. Further, the continuous energy neutron cross sections were collapsed to 238 groups using a light water reactor spectrum. A light water reactor spectrum was used to match the existing multi-group cross section libraries in the SCALE code system. The PUFF-IV module of AMPX was used to calculate the 44 group covariance matrices of the $^{63,65}$Cu neutron cross sections.

Very recent work at ORNL, by Perfetti, et al. has shown promising results for the development of a continuous energy sensitivity analysis code. [30] With such a capability, future use of the coupling methodology developed in this work will rely on continuous energy sensitivity analysis. Correspondingly, the AMPX code will only be used to calculate the continuous energy cross sections and the multi-group collapse based on a light-water reactor spectrum, discussed above, will be avoided.
2.4 Sensitivity and Uncertainty Analysis

Overview

The uncertainty analysis is usually carried out in two parts. The sensitivity of each material is evaluated in every integral benchmark experiment using the TSUNAMI module of SCALE [4]. TSUNAMI is a module of SCALE6 that is capable of calculating the sensitivity of a system's $k_{eff}$ to every isotope in the problem by using perturbation theory. The TSURFER module of the SCALE6 code package is a generalized least-squares code that can perform global differential data adjustments simultaneously to identify the data deficiencies for integral benchmark calculations. TSURFER provides the requisite quantitative information thereby identifying specific differential data changes needed to improve integral calculations. Specifically, TSURFER performs generalized linear least-squares computations for a selected set of integral experiments. In this approach, the multiplication factors, $k$-effective (integral data), are calculated using neutron transport codes with multi-group nuclear data processed from evaluated differential data. TSURFER modifies the original values of the integral measurements and the multi-group data consistent with the correlated uncertainties so that the calculated integral parameters obtained with the adjusted nuclear data agree with the adjusted experimental values, within the accuracy of first order sensitivity theory. The infinitely dilute multi-group data adjustments provide a coarse level normalization that can be incorporated into the differential data evaluation. Like, SAMMY, TSURFER minimizes the $\chi^2$ value to vary the nuclear data ($\alpha \rightarrow \alpha'$) and the measured integral responses ($m \rightarrow m'$) such that they are most consistent with their respective covariance matrices, $C_{\alpha\alpha}$ and $C_{mm}$. [34]

$$
\chi^2 = (\frac{\alpha' - \alpha}{\alpha})^T C_{\alpha\alpha}^{-1} \frac{\alpha' - \alpha}{\alpha} + (\frac{m' - m}{m})^T C_{mm}^{-1} \frac{m' - m}{m} \quad (2.16)
$$

The previous procedure for using TSURFER in differential evaluations was not coupled with the R-matrix analysis tools and did not fully take advantage of the comprehensive differential and integral analysis capabilities. In this research the
unprecedented resonance analysis capability (SAMMY) that is coupled with S/U analysis tool (TSURFER) thereby enabling the data evaluator to address specific advanced fuel cycle application needs.

The idea of using S/U analysis tools to direct differential data evaluation based on integral parameter results is not new. Research in this topic dates back more than 40 years. Ref [10] gives an example of how multi-group cross section adjustments based on integral experiment feedback were used for fast reactor applications. With the new push for better uncertainty quantification in nuclear applications in recent years, the idea of the integral data feedback is more popular than ever. However, the current methods only look to identify the areas where differential data uncertainty improvement is needed in order to improve integral results. For example, the G. Aliberti, G. Palmiotti, et al. 2006 paper [1] discusses how to identify the needed uncertainties on input nuclear data to achieve desired uncertainty for future nuclear systems application calculations.

More recently, Hoblit, et al., [15] have made progress in the field of coupling differential and integral data analysis by suggesting a methodology for systematically adjusting multi-group cross sections based feedback from sensitivity analysis of integral experiments. This technique is proposed for unifying reaction cross section libraries. Also, Palmiotti, et al., [27] have proposed a very similar method for adjusting multi-group cross sections systematically based on integral experiments. However, both of these methods go back only as far as multi-group cross sections and also generally deal with energies above the resolved resonance region. Moreover, only single-dimensional cross section data (i.e. cross section vs. energy not differential cross section with respect to angle or double differential cross section with respect to angle and energy) can be adjusted based on existing techniques. No mention of covariance updating is made anywhere in the researched literature.

This work has moved beyond identification of the areas of needed improvement and adjustment of multi-group cross sections. In the proposed methodology, systematic adjustment of the resonance parameters and covariance data is possible. The reconstructed continuous energy cross section only changes within the experimental
uncertainties in such a way as to improve both the differential and integral data fits. Furthermore, because it is the resonance parameters that are systematically changed as a consequence of the integral data feedback, the multi-dimensional cross section data (i.e. differential and double differential cross sections) are implicitly adjusted to reflect the identified inconsistencies between the differential and integral data. The systematic execution of the proposed method will be fully explained in Section 3.4.
Chapter 3

Methods

3.1 Experimental

A neutron time-of-flight setup at the MITR was used to measure the total neutron transmission through $^{63}\text{Cu}$ and $^{65}\text{Cu}$ sample targets versus TOF of the neutrons (Detailed photographs of the experimental set up are in Appendix A). Neutron bursts were created by using a cadmium chopper wheel with slit widths of 0.95 mm. The bottom $\text{D}_2\text{O}$ reflector of MITR served as the thermal neutron source (see Fig 3-1). The sample thicknesses for $^{63}\text{Cu}$ and $^{65}\text{Cu}$ were 0.0375 atoms/barn (5 mm thick) and 0.0215 atoms/barn (3 mm thick), respectively. TOF was recorded by a BF$_3$ detector located 124.46 cm from the chopper wheel. In Figure 3-2, the neutron beam comes at an angle from the direction of the viewer, passes through the pre-collimator, and then passes through the chopper wheel to begin TOF. From there, the neutron beam is attenuated by the sample and makes its way to the BF$_3$ detector at the end of the table. Finally, the beam ends up in the beam dump. A 13.5-hour run was conducted for the unattenuated beam, a 12.5-hour run was conducted for the $^{65}\text{Cu}$ sample, and an 11-hour run was conducted for the $^{63}\text{Cu}$ sample at an average reactor power of 5 MWth. The data were normalized by both the run time and the average reactor power during the run (determined to be linearly proportional to the total number of neutrons in the beam). The reactor neutron power was logged by two independent detectors in 1 minute intervals.
Figure 3-1: A schematic view of the MITR.
Figure 3-2: A schematic view of the neutron TOF experiment at MITR.
A detailed MCNP (Monte Carlo N-Particle) [7] model of the experimental set-up was created. This model was used to estimate the percent of neutrons from the beam that made first flight collisions in the detector. The neutron source distribution for the problem was obtained from a full core MCNP model of MITR.

A modification of this experimental set-up was supposed to enable the measurement of the thermal neutron radiative capture cross section. As described in Section 2.2, capture data complimentary to transmission data has no equal in value for the resolved resonance evaluation process. In principle the only major modification of the transmission set up that was needed was the installation of a gamma ray detector with gamma ray energy discrimination capability. Such a detector was installed, properly-shielded from background radiation, calibrated and tested. Several proof-of-concept experiments were successfully conducted showing the ability to record gamma rays characteristic of the \((n, \gamma)\) reaction for both \(^{63}\text{Cu}\) and \(^{65}\text{Cu}\). However, once the neutron beam flux was finally measured at the experimental beam port, it was found that the neutron flux was insufficient for capture cross section measurements with sufficient accuracy. As described in Section 2.2.1 the total neutron flux is not needed for transmission measurements and therefore was not recorded during the measurement of the total thermal cross section described above. For archival purposes, a full experimental write up is given in Appendix B, with a description of intended use for the data to be obtained, a description of the exact experimental set up and a description of the proof-of-concept experiments that were conducted.

3.2 Resolved Resonance Region Evaluation

3.2.1 Fitting of the Experimental Data

The RRR was extended by identifying new resonance energies and neutron and gamma widths. The peak search module of the ORNL code RSAP [31] was used to identity new resonances. Peak search is based on finding local maxima, minima and inflection points in the experimental data. In extending the RRR, RSAP assigns
the same user-input angular momentum to all of the newly identified resonances. The shape of the reconstructed cross section depends greatly on the quantum angular momentum of the resonances. Strictly speaking, the reconstructed cross section depends on the quantum angular momentum of all of the resonances in the evaluation because of the interference effect. Therefore, the code RSAP, does nothing more than identifying a suspected number of resonances with their approximate location in energy. The term suspected is used here to emphasize the fact that the true number of resonances cannot be deduced from realistic differential experimental data. The best a computer code can do, is identify the obvious humps in the differential data. Therefore, after RSAP finishes, the evaluator is left with a list of newly identified resonances at their respective energies.

Previously, the problem of identifying the quantum angular momentum of each resonance was once again left up to the experienced eye of the evaluator. In certain situations of excellent experimental data and with certain isotopes, it is quite easy to tell the shape of a s-wave resonance versus a p-wave resonance. However there are many factors which can ruin this idealized scenario. First, the experimental data may have such large uncertainty associated with it, that the shape of the resonance is lost. Next, there may be several different total quantum angular momenta associated with each orbital quantum angular momentum (i.e. both isotopes of copper have 2 discrete total quantum angular momenta for s-wave resonances and 6 discrete total quantum angular momenta for p-wave resonances). Further, the interference effect can distort the shape of a resonance from what it would look like without the interference effect. Lastly, double and triple resonances exist, where two or three resonances are grouped close together and produce the visual effect of a single resonance in the experimental data. An example of such a case was given in Section 2.2.

In order to address the problem of identifying the quantum angular momentum of hundreds of new resonances identified in extending the resolved resonance regions of $^{63,65}\text{Cu}$, a new wrapper code was written to select the quantum angular momentum for each resonance that would optimize the fit of the experimental data. The automated procedure steps through each resonance, one at a time, and considers a user-defined
number of quantum angular momenta possibilities for that resonance. The code runs a SAMMY case for each possibility allowing a user-defined number of nearest resonance parameters to be varied. Allowing the nearest neighbors of the resonance in question to be varied gives SAMMY enough room to adjust for the interference in the local neighborhood. After all of the allowed quantum angular momentum possibilities have been tried, the code selects the choice that results in the smallest chi-squared value for a broad energy range around the resonance in question. The concern that changing the quantum angular momentum of a resonance in one location will affect the reconstructed cross section at a different energy is addressed by the fact that the chi-squared is evaluated over a wide energy range, such that if the goodness-of-fit improved in the immediate neighborhood with the new choice for the quantum angular momentum but at the same time destroyed the fit in another energy region, the over-all chi-squared will be larger and that choice of quantum angular momentum will be rejected. In this way, the program exercises the do no harm philosophy, as in it can only improve the overall fit of the experimental data and at worst, it will return a set of resonance parameters that fit the experimental data as well as the parameters that it started with.

Currently, the program runs down the list of resonances one-by-one, in order of increasing energy. Unfortunately, this means that a resonance is being optimized considering the interference effects with resonances below it in energy (those, whose quantum angular momentum has already been determined) and resonances above it in energy (those, whose quantum angular momentum will in-turn be altered). This creates a problem in the fact that for any one resonance, the optimization is carried out based on interference effects that are not constant and may change in the future. Therefore, the code has the option of running multiple times through the list of resonances such that the interference effect between resonances can be optimized in an iterative way. The design of the code guarantees that this process will improve the goodness-of-fit until it reaches a local minimum in the optimization. At this point the evaluator can step in, fix any obvious problems in the fitting of experimental data that may take the code out of the local minimum and continue running the code,
or the evaluator may find the quantum angular momentum distribution an adequate starting point for a traditional evaluation by an experience evaluator. The code does not guarantee a global minimum and does not seek to completely replace the human evaluator. It is suggested to be simply used as a tool to jump-start the process of identifying the quantum angular momentum of new resonances.

The resolved resonance region was extended threefold from that of the ENDF/B-VII.1 evaluation, from 99.5 keV to 300 keV. The choice of extending the resolved resonance region of the new evaluation was made to give better performance in computational models with harder spectra. Extending the upper limit of the resolved resonance region to higher energies, means better performance in nuclear systems where significant portions of the neutron spectrum are in the 100 keV to 300 keV energy region and decay towards thermal energy. Such systems are typically said to have an intermediate energy spectrum. The stopping criteria for extending the resolved resonance region to higher energies was based on the resolution of the experimental data at higher energies. In the post evaluation analysis it has became evident, that 300 keV is also approximately the point of diminishing returns, as there is little to no self-shielding above 300 keV for both isotopes of copper. See discussion in Section 4.2.1.

Experimental factors such as;

- resolution function
- finite size sample
- nuclide abundances of the sample
- multiple scattering
- self-shielding
- Doppler broadening
- normalization
- background
were all calculated when evaluating the experimental data. Figure 3-3 gives an example of how important these corrections of the experimental data can be. Due to the finite size of the sample used in the experiment, the multiple scattering correction, plotted in Fig 3-3, must be added to the capture cross section. A multiple scattering correction must be applied to capture experiments to take into account neutrons that undergo one or more scattering events in the volume of the sample and ultimately terminate with a capture event before ever leaving the sample. This results in additional characteristic gamma rays being experimentally measured. Without a correction for multiple scattering an unrealistically large capture cross section is observed. For a single scattering correction, the product of the following four probabilities must be integrated over their physical limits.

1. Reaching a certain position inside the sample volume without interacting.

2. Scattering at that position into a certain solid angle.

3. Reaching a different position along the scattered direction without leaving the volume of the sample.

4. Undergoing a capture event at the new position along the scattered direction.

It is re-emphasized here, that experimental capture data has been evaluated for the first time for the two isotopes of copper. The importance of evaluating both transmission data and capture data is represented by the example in Fig 3-4. Figure 3-4 shows the state of the $^{63}$Cu evaluation after only the transmission data has been evaluated. Clearly, without an explicit evaluation of the experimental capture cross section data, it is impossible to get the capture cross section correct.

In some of the criticality safety benchmarks, such as the Zeus experiments, copper is used as a reflector material for a critical system. The large volume of the copper reflector in these experiments makes it effectively infinite in size for calculation purposes. Therefore, it is enough only to get the ratio of the capture cross section to the scattering cross section correct to satisfy the computational discrepancy of these benchmarks. However, as Fig 3-4 demonstrates, getting the ratio of the capture to
Figure 3-3: Calculated multiple scattering correction for the $^{63}\text{Cu} (n,\gamma)$ reaction.
the scattering cross section correct without evaluating experimental capture data can only be attributed to luck. If the absolute or relative value of the capture cross section carries any sensitivity in systems of intended application, both the experimental transmission data and capture data must be evaluated.¹

3.2.2 Treatment of the High Energy External Levels

The external resonances for the new evaluation were determined using a procedure described by Leal, et al. [18]. For clarity, the procedure is outlined below in point form:

1. The neutron width for each level divided by that energy level can be shown to be linear in energy across the RRR.

2. From 1, it follows that all of the resonances in the energy region of the new evaluation (let the number of identified resonances in the energy region \(0 < E < E_1\) be \(N\)) can be copied, and translated in energy to above and below the energy region of evaluation. (Therefore, there are now \(3N\) resonances between \(-E_1 < E < 2E_1\) all following the linearity relation of Point 1.)

3. The resonances in the RRR are now removed, leaving only the external resonances above and below the RRR. The effect on the RRR of the external resonances is now recorded. (i.e., The effect over \(0 < E < E_1\) from \(N\) resonances between \(-E_1 < E < 0\) and \(N\) resonances between \(E_1 < E < 2E_1\).)

4. From experience, it is known that a few external resonances are enough to reproduce the same effect in the RRR as the full set of translated resonances. Therefore, the full set of translated resonances is reduced to only a few (e.g., two) negative-energy external resonances and a dozen or so high energy external resonances. Due to the stronger interference effect of s-wave resonances over the RRR, most of the p-wave resonances are neglected from the external regions.

¹For non-fissile nuclides. For fissile nuclides, similar logic indicates that experimental transmission, capture and fission data must all be evaluated.
Figure 3-4: Plot of the capture cross section (top) and the total cross section (bottom) as reconstructed from a preliminary evaluation for $^{63}\text{Cu}$ with only the transmission data evaluated up to 300 keV. The evaluated cross section (red) is plotted on top of experimental data (green). To reduce clutter, the uncertainty on the experimental cross section is not plotted.
3.2.3 Treatment of the Negative-Energy External Levels

For isotopes with a RRR evaluation, the cross section is reconstructed from resonance parameters. This means that the value and the shape of the cross section in the thermal energy region also comes directly from the resonance parameters. The thermal cross section is most greatly influenced by the lowest energy resonances and the negative external levels. Conversely, the resonance parameters of the lowest energy resonances and the negative external resonances are most influenced in the evaluation process by the shape and value of the thermal cross section. The negative-energy external resonances received additional treatment in this evaluation due to the availability of experimental cross section data in the thermal energy region. The resonance parameters of the negative-energy external resonances were adjusted in such a way as to improve the goodness-of-fit; chi-squared value between the reconstructed cross section from the resonance parameters and the experimental data, across the thermal differential data. This contrasts the traditional practice of simply matching the thermal cross section value of the isotope at 0.0253 eV by adjusting the parameters of the external resonances. The result of including uncertainties representing the true state-of-knowledge of the thermal cross section in fitting the resonance parameters of the negative external levels is a better representation of the uncertainty on the resonance parameters.

3.2.4 Treatment of Angular Distributions

For the new resolved resonance region evaluations of $^{63,65}$Cu, the angular distributions for elastic scattering were calculated on 32 000 energy points between 1e-5 eV to 300 keV. A maximum of 7 Legendre coefficients, defined by Equation 2.14, were reported (the zeroth coefficient implicitly being unity) in the center-of-mass reference frame. In general the Legendre coefficients describing the angular distribution in the center-of-mass reference frame decay with increasing order. It was determined that Legendre coefficients of order higher than 7 were all less than 1e-8 for the two isotopes of copper. Therefore, they were not reported.
As can be seen from Figure 3-5 the Legendre coefficients clearly have a temperature dependence.

Figure 3-5 shows that the coefficient of the first Legendre polynomial changes by more than 50% between temperatures of 0 K and room temperature. With the importance of angular distributions to criticality laid out in Section 2.2 it is claimed here that to better represent physical reality, angular distributions must be temperature broadened. Section 4.3 will show that obtaining a self-consistent angular distribution is crucial to good performance of a new evaluation in benchmark calculations.

Since none of the processing codes or neutron transport codes treat the temperature dependence of angular distributions, the mathematical formulation for the temperature broadening of angular distributions is derived here.

The Leal-Hwang Doppler broadening methodology [19] can be summarized as follows. The Doppler broadened cross section, $\sigma(E, T)$, discretized as a function of energy, $E$, and temperature, $T$, can be related to the cross section at any lower temperature $T_0$ via,

$$
\sigma(E, T) = \frac{1}{E} \sum_{k=-j}^{j} a_k^j E_k \sigma(E_k, T_0)
$$

(3.1)

where $a_k^j$ are weighting coefficients to be defined below. The discrete energy points, $E_k$, chosen symmetrically around energy, $E$, such as to create a uniform grid in the square root of energy with spacing

$$
\delta v = \sqrt{\frac{1.5k_b(T - T_0)}{AWR(2j + 1)}}
$$

(3.2)

where $k_b$ is the Boltzmann constant, and $AWR$ is the ratio of the atomic weight of the target to the atomic weight of the neutron. The variable $j$ is the inverse of the size of the discretized mesh and must be chosen large enough for $a_j^j$ to be sufficiently

---

2 As to the best knowledge of the author
3 Rigorously, the Doppler broadened cross section in the Leal-Hwang methodology should be denoted as $\sigma(E_i, T_j)$ for discretized $E$ and $T$. The variable, $E_k$ in Equation 3.1 is then $E_{i+k}$. Here, the subscripts are implied.
Figure 3-5: Coefficient of Legendre polynomial of the first order for the elastic scattering angular distribution of $^{65}\text{Cu}$ as a function of energy plotted at different temperatures.
The coefficients $a_k^j$ are defined recursively as follows.

$$a_0 = \frac{2}{3}, a_1^1 = \frac{1}{6}$$  \hspace{1cm} (3.3)

$$a_j^j = \left(\frac{1}{6}\right)^j$$ \hspace{1cm} (3.4)

$$a_{j-1}^j = \frac{1}{6} a_{j-2}^{j-1} + \frac{2}{3} a_{j-1}^{j-1}$$ \hspace{1cm} (3.5)

$$a_j^0 = \frac{2}{3} a_0^{j-1} + \frac{1}{6} a_1^{j-1}$$ \hspace{1cm} (3.6)

$$a_k^j = \frac{1}{6} a_{k-1}^{j-1} + \frac{2}{3} a_k^{j-1} + \frac{1}{6} a_{k+1}^{j-1}, \text{ for } 0 < k < j - 1$$ \hspace{1cm} (3.7)

Staring from the definition of the Legendre coefficients from Section 2.2 and using the Leal-Hwang Doppler broadening formalism;

$$\alpha_l(E) = \frac{2\pi}{\sigma_s(E,T)} \int_{-1}^{+1} \sigma_s(E,T,\mu) P_l(\mu) d\mu$$ \hspace{1cm} (3.8)

Adding the temperature dependence to the Legendre coefficients, $\alpha_l(E, T)$ and substituting in the Leal-Hwang Doppler broadened cross section, one obtains,

$$\alpha_l(E, T) = \frac{2\pi \int_{-1}^{+1} \frac{1}{E} \sum_{k=-j}^{j} \frac{1}{E_k} a_k^j E_k \sigma(E_k, T, \mu) P_l(\mu) d\mu}{\sum_{k=-j}^{j} \frac{1}{E_k} a_k^j E_k \sigma(E_k, T)}$$ \hspace{1cm} (3.9)

Notice, here that the Leal-Hwang Doppler broadening methodology has been applied to both the differential and angle integrated cross sections respectively. Canceling the $1/E$ terms, and taking the summation over $k$ outside of the integral,

$$\alpha_l(E, T) = \frac{\sum_{k=-j}^{j} a_k^j E_k [2\pi \int_{-1}^{+1} \sigma(E_k, T, \mu) P_l(\mu) d\mu]}{\sum_{k=-j}^{j} a_k^j E_k \sigma(E_k, T)}$$ \hspace{1cm} (3.10)

The term in the square brackets, can be recognized as product of the Legendre coefficient of order $L$ and the angle integrated cross section at energy $E_k$ and temperature, $T_0$.

\footnote{The author sets this to be 1e-13.}
\[ \alpha_l(E, T) = \frac{\sum_{k=-j}^{j} a_k^l E_k \sigma(E_k, T_0) \alpha_l(E_k, T_0)}{\sum_{k=-j}^{j} a_k^l E_k \sigma(E_k, T_0)} \] (3.11)

Equation 3.11 defines the mathematical formalism for the temperature broadening of the angular distribution. The coefficients of Legendre polynomials at any temperature can be calculated in terms of the Legendre coefficients at an initial temperature and the angle integrated scattering cross section at the initial temperature.

3.3 Benchmarking Procedure

The product of the analysis of the available experimental data in the resonance region for the two isotopes of copper; the two new resolved resonance evaluations, were benchmarked on a set of criticality safety benchmarks from the ICSBEP. The results of this benchmarking effort were compared with the results of an identical set of benchmarks that were computed using the ENDF/B-VII.1 resonance evaluations for the two isotopes of copper. Any differences will be noted in Section 4.3.

A set of 23 benchmarks were chosen, see Table 1.2, from the ICSBEP handbook to be a representative set of criticality safety benchmarks. The benchmarks were selected such that the copper cross section would play a role in the criticality of the system. In this way, integral feedback can be acquired about the quality of the new evaluations. The benchmark models were developed in the MCNP framework. The input geometry and materials were taken directly from the experiment descriptions in the individual experimental documentation contained in the ICSBEP Handbook. The cross section libraries for all of the materials modeled in the experiments were set to ENDF/B-VII.1 for consistency.

The code SAMMY, used for the resolved resonance region evaluation, is able to output resonance parameters in the format of File 2 of the ENDF formatting system [14]. A new code was written to calculate the angular distributions based on Equation 2.14 and output them in ENDF File 4 format. The two new File 2s and File 4s were inserted into the ENDF formatted files for the two copper isotopes. The
new resolved resonance region evaluation replaced the old ones and the new angular
distributions replace the ENDF/B-VII.1 angular distributions in the energy region of
1e-5 eV to 300 keV. Any constant background reported in File 3 was removed for the
new resolved resonance region. However, all other cross sections, specifically the high
energy cross sections remained unchanged. Then, the computer code NJOY99 [21]
was used to process the new ENDF files to MCNP style continuous energy ACE (A
Compact ENDF) cross section libraries. The following modules of the NJOY99 code
were used:

1. RECONR - reconstructs resonance cross sections from resonance parameters
   and outputs to a point-wise-ENDF (PENDF) file.

2. BROADR - generates Doppler-broadened cross sections in PENDF format start-
   ing from piecewise linear cross sections in PENDF format.

3. ACER - prepares libraries in ACE format for MCNP.

The cross sections were Doppler broadened by the BROADR module to 293.6 K.
The angular distributions were initially generated at 293.6 K.

Next, the new ACE files for $^{63,65}$Cu were added to the MCNP cross section li-
braries. All of the benchmarks in Table 1.2 (see Appendix C for descriptions) were
run with the new resolved resonance region cross sections for $^{63,65}$Cu and angular
distributions calculated at 293.6 K and all other cross sections from ENDF/B-VII.1.
After, all of the benchmarks were calculated again, but now with all cross sections
from ENDF/B-VII.1. This procedure allows for a direct comparison of the effect of
the new and old resolved resonance region evaluations on the criticality of benchmark
experiments.

Additional benchmarking was done to determine the impact of the high fidelity
treatment of the angular distributions as well as the impact of temperature broad-
ening of the angular distributions. The additional benchmarks were calculated on 4
cases of the HEU-MET-INTER-006 experiment: Zeus: Intermediate-spectrum criti-
cal assemblies with a graphite-HEU core surrounded by a copper reflector. The Zeus
experiments were selected for their simple geometry and isolation of copper as the sole reflecting material. The benchmark models were calculated using a combination of the newly evaluated resolved resonance parameters and angular distributions of ENDF/B-VII.1, and then using the newly evaluated resolved resonance parameters and high fidelity angular distribution at 0 K (unbroadened).

The results of all of the benchmarking effort are presented in Section 4.3

3.4 Coupling the SAMMY and TSURFER codes: Coupled Differential and Integral Data Analysis

In the context of the life cycle of nuclear data, see Figure 2-2, the coupling of the integral data analysis to the differential data analysis introduces a new feedback mechanism which is represented by the red arrow on the left side of the schematic in Figure 3-6.

The problem of normalization of experimental data along with other systematic uncertainties, introduced in Section 1.4 and further developed in Section 2.4 is the main concern that coupling of the differential and integral data analysis is trying to address. As has been previously discussed, the systematic error from the normalization of experimental data results in an evaluation where the cross section may be too high or too low over an entire energy range. Therefore, coupling the differential (continuous energy) analysis to a multi-group code analysis tool such as TSURFER is a natural choice. It is not desired, nor would it be practical, to receive point-wise corrections from a code like TSURFER. Group-wise corrections are rather sought from information contained in the integral experiments to address systematic uncertainties in differential experimental data. For this reason, the well-established 238-group structure for criticality safety calculations was selected for this research. The level spacing of the two isotopes of copper is not so small, as it is for example in $^{238}\text{U}$, where there are an overwhelming number of resonances in each group. Figure 3-7 shows the
Figure 3-6: A flow chart showing the life cycle of nuclear data with the newly developed feedback loop shown with the red arrow on the left side of the diagram.
238 group structure superimposed on the new resonance evaluation of the $^{63}$Cu. The methodology developed here, should in principle, apply to any group structure up to a reasonably fine group structure.

For the implementation of the integral data feedback loop in this research, the energy self-shielding from continuous-energy cross sections was done using the well documented SCALE6 [4] module, CENTRUM. CENTRUM is primarily used to calculate energy self-shielding in criticality safety applications. However, the effectiveness of the proposed coupling method does depend heavily on the accuracy of the self-shielding representation. Several facts help alleviate this dependence. For one, the feedback loop should be used with multiple integral benchmark models which will have different magnitudes of energy self-shielding. Next, the feedback methodology developed in this work, will work with any self-shielding code, and different self-shielding codes can be used for comparison or multiple self-shielding codes can be used to calculate the integral data feedback. Finally, as mentioned in Section 2.3, in the near future the integral feedback methodology developed in this work will be based on continuous energy sensitivity calculations, and there will be no need for energy self-shielding models. The continuous energy sensitivities will be averaged to give group-wise sensitives to accommodate the multi-group structure of the covariance data and the TSURFER input.

After the preliminary evaluation based on the differential experimental data is judged by the evaluator to be complete, the code SAMMY is able to generate an output such that the resonance parameters and covariance data are given in ENDF format. This output file is processed through the AMPX [11] code to create SCALE Master Libraries. The Master Libraries can then be passed into the TSUNAMI tool of SCALE that is executed for each of the selected benchmark experiments and a library of TSUNAMI sensitivity data files is compiled. As a reminder, TSUNAMI calculates the sensitivity of the computed $k_{eff}$ for each of the benchmark experiments. The output of TSUNAMI is then used as input for TSURFER. As described in Section 2.4, the main part of the TSURFER output is devoted to suggested changes in the group-wise cross sections, for each group for each desired reaction based on the overall set of
Figure 3-7: 238 group structure superimposed on the new resonance evaluation of $^{63}$Cu.
benchmark experiments selected. This information can be passed into the computer code SAMMY to improve the differential evaluation by shifting the cross section to the correct place within the uncertainty bands of the differential experimental data. In principle, any measured integral quantity, not just $k_{eff}$, could be used to determine suggested group cross section changes. Precise reaction rate measurements have been used in the past to adjust multi-group cross section data. The choice of integral quantity makes no difference to the formalism of the feedback methodology developed in this work, as it begins with suggested cross section changes and operates with no knowledge of how they were obtained. For this research, feedback based on the most common measured integral quantity, $k_{eff}$, is used.

The group-wise suggested changes in the form of, $\Delta\sigma/\sigma$, are applied directly to the point-wise reconstructed cross section from the newly evaluated parameters to create a new data set. The new data set can then be used as one of the data sets in the differential analysis to re-evaluate the resonance parameters based on all of the experimental data. Now, the suggested changes based on the integral data are also included along with the original experimental differential data. The resonance parameters are then updated to reflect the suggested cross section changes based on the Bayesian updating methodology in SAMMY. As described in Section 2.2, the Bayesian updating methodology includes information from all of the experimental data sets analyzed. The new data set created based on integral benchmark feedback enters the process as yet another experimental data set.

Including the covariance data in the re-evaluation insures that the covariance data for the resonance parameters are updated systematically. If the covariance decreases as a result of this process, it means that the information in the integral benchmarks has helped in determining the correct cross section within the systematic uncertainty of the experimental data. In this case, the resonance parameters in the updated evaluation can be reported with more confidence. On the other hand, if the covariance of the resonance parameters has increased as a result of the benchmarking process, this indicates that the uncertainties reported for the differential experimental data were too large, and the information contained in the integral benchmarks support the
idea that the resonance parameters must be reported with larger uncertainties.

The new evaluation, improved by the data obtained from integral experiments, will have cross sections that reproduce the reaction cross sections within the original differential experimental data uncertainty bands, and at the same time produce updated, consistent angular distributions and covariance data.

The goal of the newly developed methodology is to enable the evaluator to reinterpret the suggested cross section changes from TSURFER to changes in the resonance parameters and covariance data of the new evaluation. In updating the resonance parameters with information from the integral experiments, the evaluator will be changing all of the reaction cross section and the differential experimental data in a consistent manner within the uncertainty bands of the experimental data. Therefore, the proof of concept for the new methodology is demonstrating the ability to adjust the resonance parameters in such a way as to reflect the suggested reaction cross section changes from TSURFER while maintaining consistency with the experimental cross sections.

The newly developed methodology for coupling of the differential and integral data analysis was applied to the two new evaluations of copper. The four Zeus experiments were used for demonstration purposes of the ability to apply the developed methodology and produce the proof-of-concept results outlined above. The four Zeus experiments were chosen because of their high sensitivity to the copper cross section in the resolved resonance region, their significant discrepancy with the model benchmark values and their simple geometry. The four Zeus benchmarks were particularly interesting because some of the cases showed an under prediction of $k_{eff}$ while other showed an over prediction when compared to the model benchmark calculations. A second set of feedback benchmarks was chosen to repeat the process to test what will happen when there is not such a significant discrepancy in $k_{eff}$ between the calculated value and the model benchmark. The two cases of LCT42 were used for this purpose. All of the selected benchmark models were then ran with the updated evaluations. Section 4.4 presents the results of applying the new coupling methodology for the new evaluation of the two isotopes of copper, as well as the changes in the benchmark
calculations.
Chapter 4

Results

4.1 Total Thermal Cross Section Measurements

After the data reduction and considering the Poisson error on the detector counts, the measured $^{63}$Cu and $^{65}$Cu total microscopic neutron cross sections were input to the SAMMY computer code. Figure 4-1 presents a plot generated by SAMMY comparing the experimental data, denoted with one standard deviation error bars (green crosses), and the evaluated total cross section (plotted as a solid red line). The new resolved resonance region parameters for both $^{63}$Cu and $^{65}$Cu were used in the SAMMY calculation. The data was reduced to give 242 energy points for $^{63}$Cu between the values of 0.00147 eV and 0.0854 eV and 217 energy points for $^{65}$Cu between 0.0130 eV and 0.0876 eV. The uncertainties on the cross section visibly increase at the lower and upper energy boundaries because of Poisson statistics. The thermal flux shape of the MITR D$_2$O reflector peaks where the uncertainty in Figure 4-1 has a minimum. A lower flux, further away from thermal flux peak results in less neutron being available in the beam at those energies. Less neutrons result in less counts being recorded and consequently greater Poisson error of the measured cross section. The count rates experienced at the energy extremes are also what determined the maximum energy range of the experimental apparatus in these measurements.

This experimental data was instrumental in determining the negative energy external levels using the methodology described in Section 3.2.3.
Figure 4-1: Plot of the thermal cross section data measured at MITR with one standard deviation uncertainty (green) versus the cross section reconstructed from the new evaluations (red). The total thermal cross section of $^{63}\text{Cu}$ is given in the top plot and $^{65}\text{Cu}$ in the bottom.
4.2 New Resolved Resonance Region Evaluation

Figure 4-2 shows the process of extending the RRR for the two isotopes of copper. The first and third plots show the evaluation as it was in the ENDF/B-VII.1 evaluation and the second and fourth plots show the final evaluation with the RRR extended to 300 keV.

Figure 4-3 compares the capture cross section in the extended resolved resonance region for both isotopes of copper before and after the new evaluation. The unphysical behavior of the ENDF/B-VII.1 evaluated capture cross section in Figure 4-3 above 60 keV is attributed to the fact that the original evaluators added an constant background correction from 60 to 99.5 keV, as discussed in Section 1.2.

Figures 4-4 through 4-7 show the new evaluation at different energies for different reaction rates in comparison with the ENDF/B-VII.1 evaluation plotted on top of experimental data. For all Figures 4-4 to 4-7, the ENDF/B-VII.1 evaluated cross section is shown in the top plot and the new evaluation evaluated cross section is shown in the bottom plot. Both the top and bottom plots have the same experimental data plotted as was used for this new evaluation. It is obvious that many new resonances have been identified in the new RRR evaluation. This will have an effect on $k_{eff}$ of any benchmark model sensitive to the copper cross section in the resonance region.

Table 4.1 presents that change in the number of resonance in the resolved resonance region between the new evaluations for $^{63,65}$Cu and the ENDF/B-VII.1 evaluation.

Table 4.2 shows the results for the ENDF/B-VII.1 evaluations for the average level spacing initially presented in Table 1.1. Now, the results of ENDF/B-VII.1 are also compared to the new evaluation.

A significant improvements has been made in identifying p-wave resonances. The new evaluation has a much closer p-wave angular momentum distribution to that reported in Mughabghab [24] than ENDF/B-VII.1. Although slight progress has been made in approaching the accepted s-wave angular momentum distribution, it was not possible to match the s-wave values reported by Mughabghab while maintaining a
Figure 4-2: New RRR evaluation versus ENDF/B-VII.1 evaluation. All four plots show the evaluated total cross section (red) plotted on top of the experimental data with one standard deviation uncertainty (green). The top two plots compare the ENDF/B-VII.1 evaluation (first plot) versus the new evaluation (second plot) for $^{63}\text{Cu}$. The bottom two plots compare the ENDF/B-VII.1 evaluation (third plot) versus the new evaluation (fourth plot) for $^{65}\text{Cu}$.

Table 4.1: Number of Resonances in $^{63,65}\text{Cu}$ Evaluations.

<table>
<thead>
<tr>
<th>Evaluation</th>
<th>$^{63}\text{Cu}$</th>
<th>$^{65}\text{Cu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Negative Energy External Levels</td>
<td>ENDF/B-VII.1 2</td>
<td>This Work 3</td>
</tr>
<tr>
<td>Resolved Resonance Region</td>
<td>221</td>
<td>1086</td>
</tr>
<tr>
<td>High Energy External Levels</td>
<td>31</td>
<td>9</td>
</tr>
<tr>
<td>Total Number of Resonances</td>
<td>254</td>
<td>1098</td>
</tr>
</tbody>
</table>
Figure 4-3: New RRR evaluation (blue) versus ENDF/B-VII.1 evaluation (red), (n,γ) reaction.

Table 4.2: Average level spacing for different angular momenta for $^{63}\text{Cu}$ and $^{65}\text{Cu}$.

<table>
<thead>
<tr>
<th>Angular Momentum</th>
<th>$^{63}\text{Cu}$</th>
<th>$^{65}\text{Cu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>s-wave</td>
<td>p-wave</td>
</tr>
<tr>
<td>Mughabghab [24]</td>
<td>722±47 eV</td>
<td>404±22 eV</td>
</tr>
<tr>
<td>ENDF/B-VII.1</td>
<td>523±53 eV</td>
<td>2268±775 eV</td>
</tr>
<tr>
<td>This Work</td>
<td>563±24 eV</td>
<td>541±26 eV</td>
</tr>
</tbody>
</table>
Figure 4-4: $^{63}$Cu (n,tot) ENDF/B-VII.1 (top) vs new evaluation (bottom). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty.
Figure 4-5: $^{63}\text{Cu}\ (n,\gamma)$ ENDF/B-VII.1 (top) vs new evaluation (bottom). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty.
Figure 4-6: $^{65}$Cu (n,tot) ENDF/B-VII.1 (top) vs new evaluation (bottom). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty.
Figure 4-7: $^{65}\text{Cu} (n,\gamma)$ ENDF/B-VII.1 (top) vs new evaluation (bottom). The evaluated cross section (red) is plotted on top of experimental data (green) shown with one standard deviation uncertainty.
A study of the s-wave scattering radius for both isotopes of copper was done. The scattering radius was introduced as a fundamental parameter of the R-Matrix model of nuclear reactions in Section 2.2. A SAMMY fitting of the s-wave scattering radius was done based on the experimental data. It was found that the most probable s-wave scattering radius for both $^{63,65}$Cu agreed with the accepted value of $6.7 \pm 0.3$ fm within the computed uncertainty. Therefore, the it is recommended that the scattering radius for both $^{63,65}$Cu remain the same as in the ENDF/B-VII.1 evaluation. The average p-wave scattering radius, unlike its s-wave counterpart, is no longer energy independent. Therefore no investigation of the average p-wave scattering radius was done.

Table 4.3 shows a comparison of the capture resonance integral, defined as,

$$I = \frac{\int_{E_1}^{E_2} \sigma \gamma / E dE}{\int_{E_1}^{E_2} 1/E dE}$$

(4.1)

where, $E$, is the energy, and $E_1$ and $E_2$ are the energy boundaries of the group in question. One standard deviation uncertainty is reported on the resonance integral calculated from the new evaluations based on the generated covariance matrices reported in Section 4.4. No uncertainty is reported on the resonance integrals calculated from the ENDF/B-VII.1 evaluations because there is no covariance data for the two isotopes of copper in the ENDF/B-VII.1 library.

### 4.2.1 Self-Shielding

The energy self-shielding factor has been calculated for the two new evaluations of copper as well as the ENDF/B-VII.1 evaluations. For the purposes of this discussion, the self-shielding factor is defined as the ratio of the energy self-shielded cross section and the un-shielded cross section. Figure 4-8 and Figure 4-9 provide plots of the self-shielding factor for the capture cross section versus background cross section for $^{63}$Cu and $^{65}$Cu respectively. The energy self-shielded cross section was calculated by NJOY assuming a typical light water reactor spectrum. The energy self-shielding factor is application dependent. The one discussed here is a suitable example for many of the
Table 4.3: Resonance integral for several energy groups for ENDF/B-VII.1 evaluation and the new evaluation for $^{63}\text{Cu}$ and $^{65}\text{Cu}$. One standard deviation uncertainty is reported on the resonance integral calculated from the new evaluation based on the new covariance data. There is no covariance data for $^{63,65}\text{Cu}$ in the ENDF/B-VII.1 library.

<table>
<thead>
<tr>
<th>Energy Boundaries</th>
<th>$^{63}\text{Cu}$ ENDF/B-VII.1</th>
<th>This Work</th>
<th>$^{63}\text{Cu}$ ENDF/B-VII.1</th>
<th>This Work</th>
<th>$^{65}\text{Cu}$ ENDF/B-VII.1</th>
<th>This Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 000</td>
<td>2.2402</td>
<td>2.2694</td>
<td>± 0.0682</td>
<td></td>
<td>0.3092</td>
<td>0.3087</td>
</tr>
<tr>
<td>17 000</td>
<td>0.0364</td>
<td>0.0278</td>
<td>± 0.0010</td>
<td></td>
<td>0.0156</td>
<td>0.0161</td>
</tr>
<tr>
<td>25 000</td>
<td>0.0633</td>
<td>0.0490</td>
<td>± 0.0018</td>
<td></td>
<td>0.0425</td>
<td>0.0326</td>
</tr>
<tr>
<td>100 000</td>
<td>0.0290</td>
<td>0.0195</td>
<td>± 0.0007</td>
<td></td>
<td>0.0177</td>
<td>0.0139</td>
</tr>
</tbody>
</table>

criticality safety benchmark calculations.

For both isotopes the general trend is the same. In the energy region of 0 keV to 50 keV the self-shielding factor is almost the same between the new evaluation and the ENDF/B-VII.1 evaluation, with the new evaluation resulting in slightly more self-shielding because several new resonances have been identified in this energy region. Even though, the ENDF/B-VII.1 evaluation goes up to 99.5 keV, a significant difference in the self-shielding factor is noticed when compared to the new evaluation over the energy region of 50 keV to 100 keV. This difference can be attributed to the non-physical capture cross section that is reconstructed from the ENDF/B-VII.1 evaluation in this energy region. A plot of the capture cross section reconstructed from the ENDF/B-VII.1 evaluation is given in Figure 4-10. Above, 100 keV, where ENDF/B-VII.1 evaluation does not have a resolved resonance evaluation. Evaluation of the new experimental data shows a significant but decreasing amount of self-shielding. Note the floating axis limits when viewing Figure 4-8 and Figure 4-9. However, both figures show that there is a significant amount of energy self-shielding above 100 keV that was not in ENDF/B-VII.1. This self-shielding effect is important for neutronics calculations. For example, in many of the LCT benchmark experiments selected for this work from the ICSBEP [5], copper has a background cross section on the order
of 10 barns. This can result in an error in the capture cross section of up to 20\%. Figure 4-8 and Figure 4-9 show that the amount of self-shielding decreases almost to zero around 300 keV, the selected upper energy bound for the resolved resonance region of the new evaluation. This justifies 300 keV as a logical upper bound in energy for criticality safety benchmarks with a light water spectrum along with being a practical upper bound due to poor experimental resolution at higher energy.

### 4.2.2 Differential Cross Section with Respect to Angle

The differential scattering cross section with respect to angle were generated for $^{63,65}$Cu from the new resolved resonance parameters at 32 000 energy points. Since copper is used as a reflector material in many criticality safety benchmark experiments, the differential scattering cross section plays an important role in determining the quality of the evaluation. The criticality of a small reflected system has large sensitivity to the angular distribution of the scattered neutrons in the reflector. Figure 4-11 shows an example of the differential scattering cross section for $^{63}$Cu at an incident neutron energy of $E = 60$ keV.

Figure 4-11 displays the traditional method of viewing the differential cross section with respect to angle. However, it is difficult to make general statements about the effects that changes in the angular distribution will make on the criticality of systems by viewing the differential cross sections in this manner. The other alternative has traditionally been to make 3-dimensional plots of the differential cross section versus energy and angle on different axes as shown in an example for the elastic scattering of carbon in Figure 4-12. However, there are two problems with the 3-dimensional visualizations. First, in this type of plot, it is very difficult to represent changes in the differential scattering cross sections or compare two differential cross sections on the same plot. Secondly, the 3-dimensional plots have been used with the low-fidelity representation of the differential scattering cross sections. The plots do the job, when the differential scattering cross sections with respect to angle are given as average cross section, smoothly varying in energy or where there are only a couple of resonances to represent. A high-fidelity model (including resonances) of
Figure 4-8: The self-shielding factor for capture for $^{63}\text{Cu}$ for the new evaluation (red) and for ENDF/B-VII.1 for six energy groups (blue). Note that the limits of the vertical axis, Self-Shielding Factor, change between different energy groups.
Figure 4-9: The self-shielding factor for capture for $^{65}\text{Cu}$ for the new evaluation (red) and for ENDF/B-VII.1 (blue) for six energy groups. Note that the limits of the vertical axis, Self-Shielding Factor, change between different energy groups.
Figure 4-10: $^{63}$Cu (n, $\gamma$) cross section from the ENDF/B-VII.1 evaluation.
the differential cross section, clutters the surface plot, making it difficult to interpret. Therefore, it is proposed to evaluate the changes in the differential cross section by plotting the coefficients of Legendre polynomials as a function of energy. For medium-weight and heavy isotopes (when the center-of-mass and laboratory frames of reference become almost identical) the coefficients, defined by Equation 2.14, of the first two polynomials, \( P_1(\mu) = \mu \) and \( P_2(\mu) = \frac{3}{2} \mu^2 - \frac{1}{2} \), have an easy physical interpretation. The first Legendre coefficient, \( \alpha_1(E) \), is often the primary determining factor of the amount of forward scattering. It determines whether more neutrons will scatter in the forward direction relative to their direction of motion or back scatter to return to where they came from. The second Legendre coefficient, \( \alpha_2(E) \), tells whether the scattering distribution of the isotope is elongated in the forward/backward direction \( (\alpha_2 > 0) \) or in the side-to-side direction \( (\alpha_2 < 0) \).

Figure 4-13 shows a plot of the first Legendre coefficient, \( \alpha_1(E) \), as a function of energy from the new evaluation of \(^{63}\text{Cu}\) versus ENDF/B-VII.1. This plot can be directly interpreted as the amount of forward scattering from \(^{63}\text{Cu}\) as a function of energy. The high fidelity representation of the angular distribution of scattering in the new evaluation reconstructs all of the naturally occurring resonances in a manner consistent with the angle integrated scattering cross section. It is also obvious from Figure 4-13 that the average behavior of the first Legendre coefficient, \( \alpha_1(E) \), is positive and larger in magnitude for the new evaluation in comparison to the ENDF/B-VII.1 evaluation. The first Legendre coefficient, \( \alpha_1(E) \), on average, positive means that the isotope, \(^{63}\text{Cu}\) is a forward scattering isotope.

Figure 4-14 shows the plot of the second Legendre coefficient, \( \alpha_2(E) \), of the angular distribution for \(^{63}\text{Cu}\). The fact that the average is greater than zero, indicates that the scattering distribution is elongated in the forward/backward direction rather than at a right angle to the direction of the incident neutron. Figure 4-15 shows the third Legendre coefficient, \( \alpha_3(E) \), of the scattering distribution. The main take-aways are the diminishing magnitude of the expansion coefficients with increasing order and the difference between the high fidelity representation of the angular distribution of the new evaluation and the average treatment of ENDF/B-VII.1.
Figure 4-11: Differential scattering cross section with respect to angle plotted at incident neutron energy of 30 keV for $^{63}$Cu.
Figure 4-12: Elastic scattering angular distribution for carbon from ENDF/B-V.
Figure 4-13: First coefficient of expansion for the angular distribution of scattering for $^{63}\text{Cu}$. 
Figure 4-14: Second coefficient of expansion for the angular distribution of scattering for $^{63}$Cu.
Figure 4-15: Third coefficient of expansion for the angular distribution of scattering for $^{63}$Cu.
4.2.3 Temperature Broadening of Angular Distribution of Scattering

The mathematical formalism derived in Section 3.2.4 for the temperature broadening of the angular distribution was tested against two temperature broadening routines implemented in the SAMMY code. SAMMY has the option of doing traditional Doppler broadening of any cross section by numerically evaluating the Doppler broadening integral or by using the Leal-Hwang methodology. SAMMY was used to Doppler broaden the differential scattering cross section to 293 K, 300 K, 600 K, 900 K, and 1200 K. From here, the temperature broadened angular distribution coefficients were calculated using the ENDF definition presented in Section 2.2. The formalism derived in Section 3.2.4 was then used with the angle integrated, unbroadened scattering cross section and the angular distribution coefficients, \( \alpha_t(E, T = 0) \) at 0 K to temperature broaden the angular distribution coefficients to the same set of temperatures. Comparing the angular distribution coefficients calculated directly from Doppler broadened differential scattering cross sections and angular distribution coefficients that were temperature broadened from coefficients at 0 K showed a matching within numerical precision. Figure 4-16 shows a sample plot comparing the temperature broadening done by SAMMY and using the direct numerical temperature broadening of the angular distribution developed in this work. Figure 4-16 shows that the derived direct temperature broadening method gives the correct result within numerical round off error. Table 4.4 gives the numerical comparison from Figure 4-16 at several energy points around the maxima and minima.

4.3 Integral Benchmark Results

The 23 benchmark cases listed in Section 1.3 and described in Appendix C were evaluated using the ENDF/B-VII.1 cross section data libraries. Analysis was made with the new evaluation for \(^{63,65}\text{Cu}\) including the scattering angular distributions at 293 K and the results are presented in Table 4.5. The last column presents the improvement
Table 4.4: Comparison of the newly developed direct temperature broadening technique for angular distributions versus computation of angular distributions from temperature broadened differential cross sections generated by SAMMY. The first Legendre coefficient, $\alpha_1(E)$, of the elastic scattering distribution for $^{65}$Cu reported.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>300 K</th>
<th>900 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>9131.0</td>
<td>-0.0505121</td>
<td>-0.0505187</td>
</tr>
<tr>
<td>9145.2</td>
<td>0.05482626</td>
<td>0.0548139</td>
</tr>
<tr>
<td>9187.4</td>
<td>-0.0284103</td>
<td>-0.0284182</td>
</tr>
<tr>
<td>9200.4</td>
<td>0.0497898</td>
<td>0.0497638</td>
</tr>
</tbody>
</table>

Figure 4.16: Comparison of the newly developed direct temperature broadening technique for angular distributions versus computation of angular distributions from temperature broadened differential cross sections generated by SAMMY. The first Legendre coefficient, $\alpha_1(E)$, of the elastic scattering distribution for $^{65}$Cu is plotted.
in benchmark calculations with the use of the new evaluations for copper. A positive value represents better integral benchmarking performance (a C/E value closer to unity) while a negative value represents poorer performance in integral benchmarking performance (a C/E value farther away from unity). An overall statistical improvement of $320 \pm 225$ pcm was noticed for the set of 23 benchmarks.

Figure 4-17 shows a study of how the capture to scattering ratio changed in LCT012 case 9 between the ENDF/B-VII.1 evaluation and the new evaluation. The capture to scattering ratio in copper was calculated for LCT012 case 9 using MCNP, energy dependent, reaction rate tallies. Figure 4-17 shows how the new evaluation reduces the capture to scattering ratio in the resolved resonance energy region. The change from the evaluation point of view came from the ability to evaluate experimental capture data. As was shown in Section 3.2, evaluating only the transmission experimental data could not have possibly led to a systematically correct determination of the capture to scattering ratio. In the case of LCT012 case 9 (see Appendix C for a description of the geometry), the copper plates are used as separation material for LEU fuel. Since, the average value of the total cross section did not change much between the ENDF/B-VII.1 evaluation and the new evaluation, the capture to scattering ratio had the most influence on the transparency of the copper separating plates to neutrons.

As discussed in Section 3.3, the four intermediate-spectrum Zeus experiments were additionally calculated with different angular distributions of elastic scattering for the two isotopes of copper. Copper cross section libraries were constructed with the angle integrated cross sections reconstructed from the new resolved resonance parameters and the scattering angular distributions from either ENDF or the high-fidelity scattering angular distribution at 0 K. The purpose of these runs was to test for the impact on $k_{eff}$ of the angular distribution of a reflector material. Figure 4-18 and Table 4.6 present the results. In both Figure 4-18 and Table 4.6, the entry labeled "ENDF/B-VII.1 Evaluation" is only given as a reference. In that case, the entire ENDF/B-VII.1 library for copper was used in the computations. The uncertainty on $k_{eff}$ of the intermediate-spectrum Zeus cases due to the stochastic nature of MCNP
Table 4.5: Computed values divided by experimental values (C/E) for 23 critical experiments containing copper. One standard deviation stochastic uncertainty is given. The last column shows the improvement (movement towards unity) in units of pcm.

<table>
<thead>
<tr>
<th>ICSBEP Name</th>
<th>ENDF/B-VII.1 Evaluation</th>
<th>New Evaluation</th>
<th>Improvement Over ENDF (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF072-01</td>
<td>1.01565 ± 0.00029</td>
<td>1.01594 ± 0.00029</td>
<td>-28 ± 41</td>
</tr>
<tr>
<td>HMI006-01</td>
<td>0.99533 ± 0.00035</td>
<td>0.99544 ± 0.00035</td>
<td>11 ± 49</td>
</tr>
<tr>
<td>HMI006-02</td>
<td>0.99593 ± 0.00035</td>
<td>0.99756 ± 0.00036</td>
<td>164 ± 50</td>
</tr>
<tr>
<td>HMI006-03</td>
<td>0.99905 ± 0.00035</td>
<td>0.99960 ± 0.00033</td>
<td>55 ± 48</td>
</tr>
<tr>
<td>HMI006-04</td>
<td>1.00589 ± 0.00030</td>
<td>1.00618 ± 0.00032</td>
<td>-29 ± 44</td>
</tr>
<tr>
<td>LCT009-10</td>
<td>0.99868 ± 0.00035</td>
<td>0.99839 ± 0.00034</td>
<td>-29 ± 49</td>
</tr>
<tr>
<td>LCT009-11</td>
<td>0.99882 ± 0.00035</td>
<td>0.99896 ± 0.00035</td>
<td>14 ± 49</td>
</tr>
<tr>
<td>LCT009-12</td>
<td>0.99979 ± 0.00036</td>
<td>0.99904 ± 0.00035</td>
<td>-75 ± 50</td>
</tr>
<tr>
<td>LCT009-13</td>
<td>0.99990 ± 0.00034</td>
<td>0.99961 ± 0.00034</td>
<td>-29 ± 48</td>
</tr>
<tr>
<td>LCT009-14</td>
<td>0.99783 ± 0.00034</td>
<td>0.99837 ± 0.00036</td>
<td>54 ± 50</td>
</tr>
<tr>
<td>LCT009-15</td>
<td>0.99946 ± 0.00034</td>
<td>0.99950 ± 0.00034</td>
<td>4 ± 48</td>
</tr>
<tr>
<td>LCT012-09</td>
<td>0.98730 ± 0.00032</td>
<td>0.98761 ± 0.00032</td>
<td>32 ± 45</td>
</tr>
<tr>
<td>LCT012-10</td>
<td>0.98878 ± 0.00033</td>
<td>0.98931 ± 0.00032</td>
<td>54 ± 46</td>
</tr>
<tr>
<td>LCT013-06</td>
<td>0.99979 ± 0.00039</td>
<td>0.99993 ± 0.00037</td>
<td>14 ± 54</td>
</tr>
<tr>
<td>LCT013-07</td>
<td>0.99926 ± 0.00037</td>
<td>0.99994 ± 0.00036</td>
<td>68 ± 56</td>
</tr>
<tr>
<td>LCT016-15</td>
<td>0.99758 ± 0.00031</td>
<td>0.99850 ± 0.00030</td>
<td>92 ± 43</td>
</tr>
<tr>
<td>LCT016-16</td>
<td>0.99561 ± 0.00031</td>
<td>0.99621 ± 0.00030</td>
<td>60 ± 43</td>
</tr>
<tr>
<td>LCT016-17</td>
<td>0.99711 ± 0.00030</td>
<td>0.99666 ± 0.00031</td>
<td>-45 ± 43</td>
</tr>
<tr>
<td>LCT016-18</td>
<td>0.99869 ± 0.00030</td>
<td>0.99800 ± 0.00031</td>
<td>-69 ± 43</td>
</tr>
<tr>
<td>LCT016-19</td>
<td>0.99915 ± 0.00030</td>
<td>0.99888 ± 0.00031</td>
<td>-27 ± 43</td>
</tr>
<tr>
<td>LCT016-20</td>
<td>0.99883 ± 0.00031</td>
<td>0.99931 ± 0.00030</td>
<td>48 ± 43</td>
</tr>
<tr>
<td>LCT042-06</td>
<td>0.99998 ± 0.00033</td>
<td>0.99977 ± 0.00033</td>
<td>-21 ± 47</td>
</tr>
<tr>
<td>LCT042-07</td>
<td>0.99893 ± 0.00033</td>
<td>0.99894 ± 0.00033</td>
<td>1 ± 47</td>
</tr>
</tbody>
</table>
Figure 4-17: Plot of the capture to scattering ratio in copper for LCT012 case 9 as a function of energy.
is very small (1σ ≈ 35 pcm). In fact, the MCNP stochastic uncertainty is smaller than the data markers in Figure 4-18. Such a small stochastic uncertainty is possible due to the small and simple geometry of these integral experiments.

The effect of using a low fidelity angular distribution that is inconsistent with the angle integrated cross section is tremendous and results in poor benchmark performance of the evaluation. Compare the entries labeled “ENDF/B-VII.1 Angular Distributions” (purple solid line) and “Angular Distributions at 293.6 K” (red solid line) where the only difference is the change of the angular distribution from the low fidelity model to the self-consistent, high fidelity model including physical resonances in the angular distributions.

Isolating the effect of only the new resolved resonance parameters for the two isotopes of copper, as opposed to looking at the new evaluations as a whole, does not paint a pretty picture. Compare the entries labeled “ENDF/B-VII.1” (blue dashed line) and “ENDF/B-VII.1 Angular Distributions” (purple solid line) where the only change is a new set of resonance parameters. The new resonance parameters, which were evaluated on 5 sets of experimental data including new experimental capture cross section measurements, appear to cause a large increase in the criticality of these benchmarks. However, the new resonance parameters in the library labeled “ENDF/B-VII.1 Angular Distributions” lead to angle integrated cross sections that are inconsistent with the angular distributions reported in the same library. Therefore, it is only correct to consider the effect on criticality of a new evaluation as a whole and not its individual pieces. Isolating parts of an evaluation results in inconsistent nuclear data and meaningless integral results. Also, it is only valid to comment

<table>
<thead>
<tr>
<th></th>
<th>HMI006-01</th>
<th>HMI006-02</th>
<th>HMI006-03</th>
<th>HMI006-04</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ang. Dist. at 293.6 K</td>
<td>0.99544</td>
<td>0.99756</td>
<td>0.99960</td>
<td>1.00618</td>
</tr>
<tr>
<td>Ang. Dist. at 0 K</td>
<td>0.99294</td>
<td>0.99661</td>
<td>1.00051</td>
<td>1.00793</td>
</tr>
<tr>
<td>ENDF/B-VII.1 Ang. Dist</td>
<td>0.99706</td>
<td>1.00143</td>
<td>1.00589</td>
<td>1.01432</td>
</tr>
<tr>
<td>ENDF/B-VII.1 Evaluation</td>
<td>0.99533</td>
<td>0.99593</td>
<td>0.99915</td>
<td>1.00589</td>
</tr>
</tbody>
</table>

Table 4.6: Computed values divided by experimental values (C/E) for the four intermediate-spectrum Zeus cases. One standard deviation stochastic uncertainty was approximately 35 pcm for all cases.
Figure 4-18: Computed values divided by experimental values (C/E) for the four intermediate-spectrum Zeus cases. For data with solid connecting lines, the angle integrated cross sections were reconstructed from the new resolved resonance region evaluation and the angular distribution of elastic scattering was used as noted in the figure legend. The data points connected with the dashed line and labeled as “ENDF/B-VII.1 Evaluation” are given as a reference and come from the calculation using the entire ENDF/B-VII.1 evaluation for copper. The thin black lines represent the model benchmark 1σ uncertainty bands.
effects on criticality and benchmarking performance of a new evaluation as a whole.

The new evaluation, as a whole, has shown improved performance evaluated on the full set of 23 benchmarks with varying geometries. Careful attention was given to obtaining the correct resonance quantum angular momentum in the new evaluations of copper. This has directly resulted in the ability to produce a set of consistent angular distributions. In this study of the effects of angular distributions it is shown that the new high fidelity angular distributions in combination with the new resonance parameters, produce superior results compared to the old evaluation.

The effect of the temperature dependence of the scattering angular distribution is evident particularly in the second and third cases of HMI006. Compare the entries labeled “Angular Distribution at 0 K” (green solid line) and “Angular Distribution at 293.6 K” (red solid line) where the only change is in the temperature at which the angular distributions of elastic scattering are reported. All of the benchmarks with the temperature broadened angular distribution were closer to the model benchmark $k_{eff}$ than the benchmarks with the unbroadened angular distribution regardless whether there was a positive or negative bias in $k_{eff}$. This implies that temperature broadening of the angular distributions of elastic scattering does not simply increase $k_{eff}$ of benchmark setups with copper as a reflector. Such a conclusion might have been drawn by observing only the first three Zeus cases, where $k_{eff}$ increased. However, the fourth Zeus case decreased in $k_{eff}$ as a consequence of the temperature broadening. This shows a motion towards the correct model benchmark $k_{eff}$ and implies a better representation of reality. The maximum observed deviation in criticality due to the temperature dependence of the scattering angular distribution was 105.6 pcm.

4.4 Results of Coupling Differential and Integral Data Analysis

The newly developed methodology for coupling of the integral data analysis with the differential evaluation was applied to two different sets of benchmarks. The four cases
of the intermediate-spectrum Zeus were used because of their potential to produce the most interesting results. The four cases of Zeus are sensitive to both the angle integrated reaction cross sections of copper and the angular distributions of elastic scattering in copper, as shown in Section 4.3. One of the advantages of coupling the integral data analysis directly to changes in the resonance parameters is the ability to change the differential reactions with respect to energy and angle (multi-dimensional nuclear data). The Zeus cases are a good choice to explore the combined impact of changing both the angle integrated cross sections (ordinary cross sections) and the differential cross sections with respect to angle. The other interesting thing about the Zeus cases, is the fact that they show a trend in increasing $k_{\text{eff}}$ and both over-shoot and under-shoot the model benchmark calculations. Along side of the four Zeus case, two LCT cases were used to test the feedback methodology.

4.4.1 Initial Covariance Data

Covariance data was generated through the SAMMY code for both of the new evaluations before the feedback methodology was applied. It is interesting to note that while the ENDF/B-VI files for $^{63,65}$Cu did include covariance data, it was removed in the transition to ENDF/B-VII. The covariance data of the two copper isotopes, along with many other nuclides, was judged to be a poor representation of the real state of knowledge of the uncertainty on the cross sections. Out of the 44 group covariance structure the first 10 (high energy) groups are above the 300 keV limit of the upper end of the resolved resonance region for the new evaluations. Until a new, high energy covariance evaluation can be done for the two isotopes of copper, there will be no high energy covariance data at these energies. Only groups 11 through 44 will be discussed here.

The generation of high energy covariance data is beyond the resolved resonance region evaluation. However, collaborative work is currently ongoing at the Karlsruhe Institute of Technology (KIT) [29], to generate high energy covariance data for the two isotopes of copper that will be consistent with the resolved resonance region covariance data generated in this work. Once, the high energy covariance evaluation
is complete, the high energy covariance data will be combined with the resolved resonance region covariance data to span the entire energy range from $1 \times 10^{-5}$ eV to 150 MeV.

Figures 4-19 and 4-20 present the calculated multi-group variances, the diagonal of the covariance matrix, for the capture cross section of $^{63}$Cu and $^{65}$Cu respectively. Tables 4.7 and 4.8 give the numerical values of the variances plotted in Figures 4-19 and 4-20 for the groups of interest in the resolved resonance region. The variances for both $^{63}$Cu and $^{65}$Cu in groups 11 to 17 show effects of the resonance region. Group 11, for both isotopes, shows a reduced variance due to the lack of high energy covariance data.

Figure 4-21 and 4-22 present the corresponding correlation matrices. Even though it may be difficult to spot the differences between correlation matrices for the two isotopes, the reader is asked to consider the difference between the horizontal (rows) and vertical (columns) bands of groups 11 through 17 that reflect the resonance behavior. The wide band of strong correlations around the major diagonal reflects the fact that cross sections in neighboring groups are stronger correlated to each other than groups far away. The fact that the correlation matrices are positive has an intuitive physical interpretation. If the cross section in one group was to increase the cross sections in the other groups would also increase.

The calculated multi-group variances, the diagonal of the covariance matrix, for elastic scattering cross section of $^{63,65}$Cu are presented in Tables 4.9 and 4.10. The covariance data of the elastic scattering reaction for both isotopes of copper is almost

<table>
<thead>
<tr>
<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>100 000 - 400 000</td>
<td>2.8964</td>
</tr>
<tr>
<td>12</td>
<td>25 000 - 100 000</td>
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</tr>
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</tr>
<tr>
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<td>17 000 - 3 000</td>
<td>3.1698</td>
</tr>
<tr>
<td>15</td>
<td>3 000 - 550</td>
<td>3.0003</td>
</tr>
<tr>
<td>16</td>
<td>550 - 100</td>
<td>3.2050</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>3.0206</td>
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Table 4.8: $^{65}\text{Cu}$ (n,$\gamma$) relative standard deviation; the diagonal of the covariance matrix.

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<th>Energy Boundaries (eV)</th>
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</thead>
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<tr>
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</tr>
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</tr>
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</tr>
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<td>16</td>
<td>550 - 100</td>
<td>3.1562</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>3.0017</td>
</tr>
</tbody>
</table>

Figure 4-19: $^{63}\text{Cu}$ (n,$\gamma$) relative standard deviation; the diagonal of the covariance matrix. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{63}\text{Cu}$. 
Figure 4-20: $^{65}\text{Cu} (n,\gamma)$ relative standard deviation; the diagonal of the covariance matrix. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{65}\text{Cu}$.
Figure 4-21: $^{63}\text{Cu} (n,\gamma)$ correlation matrix. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{63}\text{Cu}$. 
Figure 4-22: $^{65}$Cu (n,γ) correlation matrix. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{65}$Cu.
completely dominated by the potential scattering. Therefore, not much of the effect of the resonances can be seen in the variance data for the elastic scattering reaction. Similar to the capture reaction discussed above, group 11 for the scattering covariance matrix, suffers from a lack of high energy covariance data.

### 4.4.2 Results of Resonance Parameter Adjustments Based on Analysis of Intermediate-Spectrum Zeus Integral Experiments

As discussed in Section 3.4 the TSUNAMI and TSURFER modules of the SCALE code system were executed to obtain the suggested reaction cross section changes for the Zeus experiments. The reader is reminded that the code TSURFER suggests cross section changes for all of the reactions, for every energy group, for all of the isotopes in the integral systems analyzed. Table 4.11 presents a small sample of some of the suggested cross section changes based on the analysis of the four Zeus benchmarks. The correct interpretation of the output of TSURFER is that if all of the suggested cross section changes are made, the integral benchmark calculated $k_{eff}$ will line up with the model benchmark values. However, in this work, the reaction cross section only for the two isotopes of copper are changed. Therefore, a significant improvement in benchmark calculations is not expected.

Figures 4-23 and 4-24 present the suggested changes to the capture cross section

<table>
<thead>
<tr>
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<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
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<td>2.0001</td>
</tr>
<tr>
<td>12</td>
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<tr>
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<td>17 000 - 3 000</td>
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<td>3.0001</td>
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<td>16</td>
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<td>100 - 30</td>
<td>3.0008</td>
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<tr>
<td>18</td>
<td>30 - 10</td>
<td>3.003</td>
</tr>
<tr>
<td>19 - 44</td>
<td>10 - 0.00001</td>
<td>3.0002</td>
</tr>
</tbody>
</table>
Table 4.10: $^{65}$Cu (n,els) relative standard deviation; the diagonal of the covariance matrix.

<table>
<thead>
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<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
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<td>2.0007</td>
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<tr>
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<td>30 - 10</td>
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</tr>
<tr>
<td>19 - 44</td>
<td>10 - 0.00001</td>
<td>3.0004</td>
</tr>
</tbody>
</table>

Table 4.11: Examples of suggested cross section changes from the Zeus integral benchmark feedback. A sampling of reactions, energy groups and isotopes is presented. The full TSURFER output consists of suggested changes for all reactions, all energy groups and all isotopes.
based on the integral data feedback from the four Zeus cases. The suggested cross section changes are plotted as relative changes and compared in magnitude to the calculated relative standard deviation for the capture cross sections. For the four Zeus cases, the TSURFER calculations suggest a decrease in the capture cross section for both isotopes of copper. Therefore, the suggested relative changes are negative. In order to facilitate an easier comparison, the relative standard deviation is plotted as a negative value in Figures 4-23 and 4-24. Figures 4-25 and 4-26 show the suggested changes in the (angle integrated) elastic scattering cross section based on feedback from the integral Zeus experiments. The calculated variance for the elastic scattering cross section is given in the same plots for comparison.

As expected, the cross section changes suggested by TSURFER are almost constant across the entire energy range. This is because most of the stochastic uncertainty in the cross sections is eliminated in the evaluation process and the systematic uncertainty is what remains. As discussed previously, such experimental systematic uncertainty mostly comes from normalization and background. The fact that TSURFER suggests an almost constant cross section change across the entire resolved resonance region support this assertion. As evidenced by Figures 4-23 through 4-24, TSURFER suggests only small changes in the copper cross sections. Although this cannot be used as proof of the fact, it does suggest that the new evaluation of the two copper isotopes is accurate.

The suggested cross section changes were then used to create new data sets for the SAMMY fitting process. A capture cross section data set and a scattering cross section data set were created based on the Zeus integral benchmark feedback. These two data sets were then used to update the resonance parameters and covariance matrices for new evaluations of the two isotopes of copper through the SAMMY fitting process discussed in Section 2.2. An updated set of resolved resonance region evaluations for $^{63,65}$Cu based on the Zeus feedback was created.

Figures 4-27 through 4-30 present results of the resonance parameter adjustment process based on the feedback from the Zeus criticality safety integral benchmarks. The results are presented in the same style as the suggested cross section changes
Figure 4-23: Suggested relative changes for $^{63}\text{Cu} \,(n,\gamma)$ cross section (red) based on feedback from the Zeus integral experiments and computed relative standard deviation (plotted as negative) on the $^{63}\text{Cu} \,(n,\gamma)$ cross section (green) from Figure 4-19. The relative standard deviation is plotted as negative to allow for a visual boundary for the suggested cross section changes from TSURFER. The vertical axis is dimension-less; the values represent the percent of the quantity in question. For example, a 4 value represents 4% of the capture cross section.
Figure 4-24: Suggested relative changes for $^{65}$Cu (n,γ) cross section (red) based on feedback from the Zeus integral experiments and computed relative standard deviation (plotted as negative) on the $^{65}$Cu (n,γ) cross section (green) from Figure 4-20. The relative standard deviation is plotted as negative to allow for a visual boundary for the suggested cross section changes from TSURFER. The vertical axis is dimension-less; the values represent the percent of the quantity in question. For example, a -4 value represents 4% of the capture cross section.
Figure 4-25: Suggested relative changes for $^{63}$Cu (n,els) cross section (red) based on feedback from the Zeus integral experiments and computed relative standard deviation (plotted as negative) on the $^{63}$Cu (n,els) cross section (green). The vertical axis is dimension-less; the values represent the percent of the quantity in question. For example, a 4 value represents 4% of the elastic scattering cross section.
Figure 4-26: Suggested relative changes for $^{65}$Cu (n,els) cross section (red) based on feedback from the Zeus integral experiments and computed relative standard deviation (plotted as negative) on the $^{65}$Cu (n,γ) cross section (green). The vertical axis is dimension-less; the values represent the percent of the quantity in question. For example, a 4 value represents 4% of the elastic scattering cross section.
above, Figures 4-23 through 4-35. Figures 4-27 through 4-30 were obtained through a comparison of the reconstructed cross sections from the unadjusted resonance parameters with the reconstructed cross sections from the adjusted resonance parameters. The plots present the difference between the two cross sections normalized by the magnitude of the unadjusted cross section. In pseudo-equation form, it is,

\[
\text{plotted result} = \frac{(\text{adjusted cross section} - \text{unadjusted cross section}) \times 100\%}{\text{unadjusted cross section}}
\]  

(4.2)

This style is presented to show proof of the ability to make the suggested cross section changes from TSURFER via adjustment of the resonance parameters directly. Several observations can be made from Figures 4-27 through 4-30. First, the suggested cross section changes are reflected in the reconstructed cross sections in an average manner. The significant amount of oscillation around the average change in the cross section comes from two sources. The cross section adjustment having been made through the resonance parameters is reflected by some of the resonance structure coming out in the relative difference between the adjusted and unadjusted cross sections. The second source of oscillations is an intrinsic problem of the definition of relative change. If the denominator in Equation 4.2 is small, the reported relative change is large. This leads to a discussion of the clearly visible group boundary at 100 keV in Figure 4-27. It is argued here, that it is exactly because the adjustment of the cross sections is made directly through the resonance parameters that the group boundary issue is not reflected in the reconstructed cross sections. The feature in Figure 4-27 is an unfortunate artifact of the presentation style of relative change in the cross sections. Figure 4-31 supports this claim. Figure 4-31 shows the difference taken directly between the adjusted and unadjusted cross sections at the energy boundary displays smooth behavior. Furthermore, the absolute magnitude of the capture cross section for the two isotopes of copper is quite small in the resolved resonance region as can be deduced from a comparison of Figures 4-2 and 4-3. This is also illustrated in the example of Figure 4-17 with the discussion of the capture to
scattering ratio. The small value of the capture cross section brings out the group boundary effect in the plots of the relative changes in the capture cross section. Note, that for the larger elastic scattering cross section, no energy group boundaries are visible in Figures 4-29 and 4-30 and the average behavior is smooth across the entire resolved resonance energy region.

The coupling methodology of differential and integral data analysis presented here, offers the advantage of adjusting the multi-dimensional cross section data through the updating of the resonance parameters. In this case, changes in the resonance parameters are reflected in the angular distributions of elastic scattering. Figures 4-32 and 4-33 present the changes in the angular distributions for $^{63}\text{Cu}$ and $^{65}\text{Cu}$ respectively. In light of previous discussions, the changes in angular distributions are presented as changes in the first Legendre coefficient of expansion. Due to the fact that the first Legendre coefficient, $\alpha_1(E)$, as a function of energy crosses the zero value many times, the relative change is not given. The absolute change in the first coefficient is given instead and the reader is referred back to Figure 4-13 for an idea of the magnitude of the first Legendre coefficient for elastic scattering in the resolved resonance range. The plotted changes in the angular distributions are not on a relative scale, therefore, all of the complex oscillating behavior is directly associated with physical resonances. Furthermore, a slight general trend of increasing the first Legendre coefficient can be noticed in both plots. As has been previously discussed, this can be interpreted as an overall increase in forward scattering.

In summary, the new evaluations updated based on integral data feedback from the Zeus cases have resulted in an increased elastic scattering cross section across the resolved resonance region and in a slightly decreased scattering cross section. Tracing back to the differential experimental data, this can be interpreted as a change in the normalization of the experimental capture data within the reported experimental uncertainty. The combined effect is a slightly decreased capture to scattering ratio. Finally, the updated angular distribution points to a very slight increase in the amount of forward scattering by both isotopes.

The processing steps discussed in Section 2.3 and benchmarking steps discussed
Figure 4-27: Relative changes for $^{63}\text{Cu} \ (n,\gamma)$ cross section made based on feedback from the Zeus integral experiments directly through adjustment of resonance parameters.
Figure 4-28: Relative changes for $^{65}\text{Cu} \ (n,\gamma)$ cross section made based on feedback from the Zeus integral experiments directly through adjustment of resonance parameters.
Figure 4-29: Relative changes for $^{63}\text{Cu} (\text{n,els})$ cross section made based on feedback from the Zeus integral experiments directly through adjustment of resonance parameters.
Figure 4-30: Relative changes for $^{65}$Cu (n,els) cross section made based on feedback from the Zeus integral experiments directly through adjustment of resonance parameters.
Figure 4-31: Difference between the adjusted and unadjusted $^{63}$Cu (n,$\gamma$) cross section. This figure presents the results shown in Figure 4-27 around 100 keV. Here, the results are plotted as the difference rather than the relative difference, as in Figure 4-27. It is evident that the abrupt jump seen in Figure 4-27 is a numerical artifact.
Figure 4-32: Changes in the first Legendre coefficient for the angular distribution of elastic scattering in $^{63}$Cu made based on feedback from the Zeus integral experiments directly through adjustment of resonance parameters. The vertical axis is dimensionless.
Figure 4-33: Changes in the first Legendre coefficient for the angular distribution of elastic scattering in $^{65}$Cu made based on feedback from the Zeus integral experiments directly through adjustment of resonance parameters. The vertical axis is dimensionless.
in Section 3.3 were repeated for the updated evaluations. Figure 4-34 shows the benchmarking results for the four intermediate-spectrum Zeus cases using the new evaluation updated based on the integral feedback obtained from those same cases. Only small changes in $k_{eff}$ of the four cases were observed. All of the changes were within two standard deviations, therefore, a clear cut improvement in the benchmark calculations cannot be argued. However, this is not unexpected. Small changes in $k_{eff}$ in response to updates of the copper evaluations were foreshadowed by the small magnitude of the cross section changes suggested by TSURFER. As has been previously discussed, TSURFER had already allocated much of the discrepancy between the calculated and benchmark model $k_{eff}$ to the other isotopes in the problem. Furthermore, the combined capabilities of TSUNAMI and TSURFER do not allow the current sensitivity/uncertainty analysis methodology to evaluate the impact of changing angular distributions of elastic scattering on the criticality of integral systems. As will be discussed in the concluding chapter of this work, multi-dimensional nuclear data sensitivity/uncertainty analysis is a good topic for future research originating from this work.

The performance of the updated evaluation based on the Zeus integral data feedback on the entire set of 23 benchmark experiments selected for this work is presented in Table 4.12. Once again, the relatively small suggested cross section changes do not lead to statistically identifiable changes in $k_{eff}$ of the selected benchmarks. The bottom rows of Table 4.12 present the statistical analysis.

4.4.3 Results of Resonance Parameter Adjustments Based on Analysis of LCT042 Integral Experiments

The TSUNAMI and TSURFER modules of the SCALE code system were executed to obtain the suggested reaction cross section changes for the LCT042 experiments. The TSURFER calculation for the two LCT042 cases produced an entirely different result than the Zeus cases. When the sensitivity/uncertainty analysis was applied on the two LCT042 benchmarks, TSURFER found it necessary only to change the
Figure 4-34: Computed values divided by experimental values (C/E) for the four intermediate-spectrum Zeus cases. The thin black lines represent the model benchmark 1σ uncertainty bands. The "Updated Evaluation" was updated based on the integral data feedback from the four intermediate-spectrum Zeus cases, HMI006.
Table 4.12: Computed values divided by experimental values (C/E) for 23 critical experiments containing copper. One standard deviation stochastic uncertainty is given. The “Updated Evaluation” was updated based on the integral data feedback from the four intermediate-spectrum Zeus cases, HMI006. The last two columns show the improvement (movement towards unity) in units of pcm. “New” refers to the new evaluation based only on differential experimental data.

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<th>ICSBEP Name</th>
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<th>Improvement New vs. ENDF (pcm)</th>
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</thead>
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</tr>
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<td>202 ± 96</td>
<td></td>
</tr>
<tr>
<td>LCT</td>
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<td>146 ± 199</td>
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</tbody>
</table>
$^{63}\text{Cu } (n,\gamma)$ reaction cross section. According to the calculations, the other three reaction cross sections, $^{63}\text{Cu } (n,\text{els})$, $^{65}\text{Cu } (n,\gamma)$ and $^{65}\text{Cu } (n,\text{els})$, required relative changes of less than 0.001%. The interpretation of these results is that the sensitivity/uncertainty analysis suggests that the discrepancy of 23 pcm left in the LCT042 case 06 and 106 pcm left in the LCT042 case 07 after the use of the new copper evaluations comes from the nuclear data of the other isotopes in these benchmarks or partially from the high energy evaluation of the two isotopes of copper. Nevertheless, the suggested capture cross section changes for $^{63}\text{Cu}$ were analyzed and revealed some interesting things about cross section adjustments directly through resonance parameters. Figure 4-35 shows the relative capture cross section adjustment suggested by TSURFER. Note the changed scale of the vertical axis.

For the updating of the resolved resonance parameters of $^{63}\text{Cu}$, only a capture cross section data set was created based on the feedback from the LCT042 integral benchmarks. The capture data set associated with LCT042 was then used to update the resonance parameters and covariance matrices of the new $^{63}\text{Cu}$ evaluation through the SAMMY fitting procedure.

Figure 4-36 presents the results of the resonance parameter adjustments based on feedback from the LCT042 integral benchmarks sensitivity/uncertainty analysis. The results of adjusting the resonance parameters are reflected in the changes in the reconstructed capture cross section.

The processing steps discussed in Section 2.3 and benchmarking steps discussed in Section 3.3 were repeated for the updated evaluation. The new evaluation updated based on the two LCT042 cases, to no surprise, did not lead to any statistically significant changes in $k_{\text{eff}}$ of any of the 23 benchmarks selected for this work. The changes in the capture cross section of $^{63}\text{Cu}$ were too small to be witnessed with the observed stochastic uncertainty of the integral calculations. The results are presented for completeness in Table 4.13.
Figure 4-35: Suggested relative changes for $^{63}\text{Cu} \ (n,\gamma)$ cross section based on feedback from the LCT042 integral experiments. The vertical axis is dimension-less; the values represent the percent of the quantity in question. For example, a 0.001 value represents 0.001% of the capture cross section. In comparison to Figures 4-23 through 4-26 note the changed scale of the vertical axis.
Figure 4-36: Relative changes for $^{63}\text{Cu} \,(n,\gamma)$ cross section made based on feedback from the LCT042 integral experiments directly through adjustment of resonance parameters.
Table 4.13: Computed values divided by experimental values (C/E) for 23 critical experiments containing copper. One standard deviation stochastic uncertainty is given. The “Updated Evaluation” was updated based on the integral data feedback from the two LCT042 cases. The last two columns show the improvement (movement towards unity) in units of pcm. “New” refers to the new evaluation based only on differential experimental data.

<table>
<thead>
<tr>
<th>ICSBEP Name</th>
<th>Updated Evaluation</th>
<th>Improvement New vs. Updated (pcm)</th>
<th>Improvement New vs. ENDF (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF072-01</td>
<td>1.01504 ± 0.00030</td>
<td>-1 ± 42</td>
<td>-28 ± 41</td>
</tr>
<tr>
<td>HMI006-01</td>
<td>0.99331 ± 0.00036</td>
<td>16 ± 50</td>
<td>11 ± 49</td>
</tr>
<tr>
<td>HMI006-02</td>
<td>0.99773 ± 0.00034</td>
<td>7 ± 50</td>
<td>164 ± 50</td>
</tr>
<tr>
<td>HMI006-03</td>
<td>1.00102 ± 0.00034</td>
<td>-8 ± 47</td>
<td>55 ± 48</td>
</tr>
<tr>
<td>HMI006-04</td>
<td>1.00691 ± 0.00034</td>
<td>87 ± 47</td>
<td>-29 ± 44</td>
</tr>
<tr>
<td>LCT009-10</td>
<td>0.99881 ± 0.00035</td>
<td>42 ± 49</td>
<td>-29 ± 49</td>
</tr>
<tr>
<td>LCT009-11</td>
<td>0.99842 ± 0.00035</td>
<td>-54 ± 49</td>
<td>14 ± 49</td>
</tr>
<tr>
<td>LCT009-12</td>
<td>1.00011 ± 0.00035</td>
<td>85 ± 49</td>
<td>-75 ± 50</td>
</tr>
<tr>
<td>LCT009-13</td>
<td>1.00024 ± 0.00036</td>
<td>15 ± 50</td>
<td>-29 ± 48</td>
</tr>
<tr>
<td>LCT009-14</td>
<td>0.99856 ± 0.00035</td>
<td>19 ± 50</td>
<td>54 ± 50</td>
</tr>
<tr>
<td>LCT009-15</td>
<td>0.99981 ± 0.00034</td>
<td>31 ± 48</td>
<td>4 ± 48</td>
</tr>
<tr>
<td>LCT012-09</td>
<td>0.98755 ± 0.00032</td>
<td>-6 ± 45</td>
<td>32 ± 45</td>
</tr>
<tr>
<td>LCT012-10</td>
<td>0.98967 ± 0.00033</td>
<td>37 ± 46</td>
<td>54 ± 46</td>
</tr>
<tr>
<td>LCT013-06</td>
<td>1.00043 ± 0.00037</td>
<td>-3 ± 52</td>
<td>14 ± 54</td>
</tr>
<tr>
<td>LCT013-07</td>
<td>0.99970 ± 0.00035</td>
<td>-24 ± 50</td>
<td>68 ± 52</td>
</tr>
<tr>
<td>LCT016-15</td>
<td>0.99775 ± 0.00030</td>
<td>-75 ± 42</td>
<td>92 ± 43</td>
</tr>
<tr>
<td>LCT016-16</td>
<td>0.99517 ± 0.00031</td>
<td>-105 ± 43</td>
<td>60 ± 43</td>
</tr>
<tr>
<td>LCT016-17</td>
<td>0.99686 ± 0.00030</td>
<td>20 ± 43</td>
<td>-45 ± 43</td>
</tr>
<tr>
<td>LCT016-18</td>
<td>0.99873 ± 0.00030</td>
<td>73 ± 43</td>
<td>-69 ± 43</td>
</tr>
<tr>
<td>LCT016-19</td>
<td>0.99829 ± 0.00031</td>
<td>-59 ± 44</td>
<td>-27 ± 43</td>
</tr>
<tr>
<td>LCT016-20</td>
<td>0.99867 ± 0.00031</td>
<td>-64 ± 43</td>
<td>48 ± 43</td>
</tr>
<tr>
<td>LCT042-06</td>
<td>1.00010 ± 0.00032</td>
<td>13 ± 46</td>
<td>-21 ± 47</td>
</tr>
<tr>
<td>LCT042-07</td>
<td>0.99847 ± 0.00034</td>
<td>-47 ± 47</td>
<td>1 ± 47</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>-34 ± 225</td>
<td>320 ± 225</td>
</tr>
<tr>
<td>All</td>
<td></td>
<td>102 ± 97</td>
<td>202 ± 96</td>
</tr>
<tr>
<td>HMI</td>
<td></td>
<td>-135 ± 199</td>
<td>146 ± 199</td>
</tr>
<tr>
<td>LCT</td>
<td></td>
<td>-34 ± 66</td>
<td>-20 ± 66</td>
</tr>
<tr>
<td>LCT042</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
4.4.4 Discussion of Covariance Updating

The final piece of the application of the newly established coupling methodology is the updating of the covariance data. It is important to note that the updated covariance data reported here has been generated only for the purpose of demonstrating how the methodology works. It is by no means proposed to submit the updated covariance data for the two copper evaluations to a national nuclear data repository, such as ENDF, after being updated on merely a few integral experiments. The four Zeus experiments were used only to prove that the newly developed concept works; that it is possible to use the information contained in integral benchmarks to systematically adjust the resonance parameters and the covariance data. In fact, two different sets of covariance data are presented further, one based on updates from the Zeus experiments and one based on updates from the LCT042 experiments. The practical application of the coupling methodology developed in this work should be used with feedback from a large assortment of integral benchmark experiments of different geometries, materials and reactor physics characteristics. The two different versions of the covariance data presented here serve as examples of what the updated covariance data would look like assuming that the TSURFER suggested cross sections reported above came from an analysis of a wide variety of integral experiments.

4.4.5 Updated Covariance Data Based on Analysis of Intermediate-Spectrum Zeus Integral Experiments

The updated covariance data based on the feedback from the four cases of the intermediate-spectrum Zeus benchmark is presented in Figures 4-37 through 4-40 in a manner similar to how the covariance data was first introduced in this section. Figure 4-37 shows the diagonal of the updated covariance matrix for the $^{63}$Cu ($n,\gamma$) reaction with the diagonal of the original, from Figure 4-19, plotted for reference. Table 4.14 supports Figure 4-37 with the numerical values. The updated resonance parameters result in a different structure of the covariance data in the resonance region. The updated correlation matrix for the ($n,\gamma$) reaction in $^{63}$Cu is given in
Figure 4-39. Figure 4-38 shows the diagonal of the covariance matrix for the \(^{65}\text{Cu}\) (n,\(\gamma\)) reaction with the diagonal of the original, from Figure 4-20. The associated numerical values are reported in Table 4.15. It is interesting to note here, that the updated resonance parameters for \(^{65}\text{Cu}\) show almost no structure in resonance groups. The updated correlation matrix for the (n,\(\gamma\)) reaction in \(^{65}\text{Cu}\) is given in Figure 4-40.

Tables 4.16 and 4.17 present the changes to the diagonal of the elastic scattering covariance matrix for \(^{63,65}\text{Cu}\) respectively. An increased amount of certainty (decreased variance) associated with the application of the knowledge from the integral data analysis is noted in the variances.

### 4.4.6 Updated Covariance Data Based on Analysis of LCT042 Integral Experiments

The original set of covariance data, presented in the beginning of this section, was updated based on the integral data feedback from the two LCT042 experiments. The sensitivity/uncertainty analysis of the two LCT042 cases suggested almost no cross section changes. The updated diagonal of the capture covariance matrix for \(^{63}\text{Cu}\) is presented in Figure 4-41 and Table 4.18. The overall effect has been a decrease in the covariance data. Further, the characteristic resonance structure has disappeared almost entirely. The correlation matrix, presented in Figure 4-42, has lost most of its off-diagonal structure as well.

Table 4.14: \(^{63}\text{Cu}\) (n,\(\gamma\)) relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments.

<table>
<thead>
<tr>
<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>100 000 - 400 000</td>
<td>3.1498</td>
</tr>
<tr>
<td>12</td>
<td>25 000 - 100 000</td>
<td>4.2670</td>
</tr>
<tr>
<td>13</td>
<td>17 000 - 25 000</td>
<td>4.2520</td>
</tr>
<tr>
<td>14</td>
<td>17 000 - 3 000</td>
<td>3.1803</td>
</tr>
<tr>
<td>15</td>
<td>3 000 - 550</td>
<td>2.9993</td>
</tr>
<tr>
<td>16</td>
<td>550 - 100</td>
<td>3.2046</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>3.0196</td>
</tr>
</tbody>
</table>
Table 4.15: $^{65}\text{Cu} (n,\gamma)$ relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments.

<table>
<thead>
<tr>
<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>100 000 - 400 000</td>
<td>2.0007</td>
</tr>
<tr>
<td>12</td>
<td>25 000 - 100 000</td>
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<td>17 000 - 25 000</td>
<td>3.0011</td>
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<td>14</td>
<td>17 000 - 3 000</td>
<td>3.0011</td>
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<tr>
<td>15</td>
<td>3 000 - 550</td>
<td>3.0014</td>
</tr>
<tr>
<td>16</td>
<td>550 - 100</td>
<td>3.1572</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>3.0031</td>
</tr>
</tbody>
</table>

Figure 4-37: $^{63}\text{Cu} (n,\gamma)$ relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{63}\text{Cu}$.
Figure 4-38: $^{65}$Cu (n,γ) relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{65}$Cu.

Table 4.16: $^{63}$Cu (n,els) relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments.

<table>
<thead>
<tr>
<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>100 000 - 400 000</td>
<td>1.9974</td>
</tr>
<tr>
<td>12</td>
<td>25 000 - 100 000</td>
<td>2.9961</td>
</tr>
<tr>
<td>13</td>
<td>17 000 - 25 000</td>
<td>2.9962</td>
</tr>
<tr>
<td>14</td>
<td>17 000 - 3 000</td>
<td>2.9961</td>
</tr>
<tr>
<td>15</td>
<td>3 000 - 550</td>
<td>2.9961</td>
</tr>
<tr>
<td>16</td>
<td>550 - 100</td>
<td>2.9977</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>2.9968</td>
</tr>
<tr>
<td>18</td>
<td>30 - 10</td>
<td>2.9963</td>
</tr>
<tr>
<td>19 - 44</td>
<td>10 - 0.00001</td>
<td>2.9962</td>
</tr>
</tbody>
</table>
Figure 4-39: $^{63}\text{Cu} \ (n,\gamma)$ correlation matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{63}\text{Cu}$.

Table 4.17: $^{65}\text{Cu} \ (n,\text{els})$ relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments.

<table>
<thead>
<tr>
<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>100 000 - 400 000</td>
<td>1.9987</td>
</tr>
<tr>
<td>12</td>
<td>25 000 - 100 000</td>
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</tr>
<tr>
<td>13</td>
<td>17 000 - 25 000</td>
<td>2.9980</td>
</tr>
<tr>
<td>14</td>
<td>17 000 - 3 000</td>
<td>2.9981</td>
</tr>
<tr>
<td>15</td>
<td>3 000 - 550</td>
<td>2.9982</td>
</tr>
<tr>
<td>16</td>
<td>550 - 100</td>
<td>2.9982</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>2.9981</td>
</tr>
<tr>
<td>18</td>
<td>30 - 10</td>
<td>2.9981</td>
</tr>
<tr>
<td>19 - 44</td>
<td>10 - 0.00001</td>
<td>2.9981</td>
</tr>
</tbody>
</table>
Figure 4-40: $^{65}$Cu (n,γ) correlation matrix. This covariance data has been updated based on the integral data feedback from the four Zeus experiments. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{65}$Cu.

Table 4.18: $^{63}$Cu (n,γ) relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the two LCT042 experiments.

<table>
<thead>
<tr>
<th>Group Number</th>
<th>Energy Boundaries (eV)</th>
<th>Standard Deviation (%)</th>
</tr>
</thead>
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<td>12</td>
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<td>13</td>
<td>17 000 - 25 000</td>
<td>3.0000</td>
</tr>
<tr>
<td>14</td>
<td>17 000 - 3 000</td>
<td>3.0000</td>
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<td>15</td>
<td>3 000 - 550</td>
<td>3.0000</td>
</tr>
<tr>
<td>16</td>
<td>550 - 100</td>
<td>3.0443</td>
</tr>
<tr>
<td>17</td>
<td>100 - 30</td>
<td>3.0206</td>
</tr>
</tbody>
</table>
Figure 4-41: $^{63}\text{Cu} \ (n,\gamma)$ relative standard deviation; the diagonal of the covariance matrix. This covariance data has been updated based on the integral data feedback from the two LCT042 experiments. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{63}\text{Cu}$. 

Before Adjustment

After Adjustment
Figure 4-42: $^{63}$Cu (n,γ) correlation matrix. This covariance data has been updated based on the integral data feedback from the two LCT042 experiments. Only groups 11 through 44 are plotted because there is no high energy covariance data for $^{63}$Cu.
4.4.7 Impact of New Coupling Methodology

The results presented in this section show that the newly developed methodology is capable of achieving the objectives laid out in Section 3.4. Despite the fact that changes in the copper evaluations did not lead to statistically improved benchmark performance, the nuclear data adjustment capabilities have been clearly demonstrated. It was shown that based on the feedback from integral data it is possible to adjust the resolved resonance parameters in such a way as to reflect the suggested cross section changes. Figures 4-27 through 4-36 show this capability. The self consistency in the reconstructed cross sections is guaranteed by the changes being applied to the resonance parameters directly. Further, in Figures 4-32 and 4-33, it was shown, for the first time, how multi-dimensional cross section data is adjusted based on integral data analysis. Finally, it was demonstrated how the covariance data for the resolved resonance region evaluation can be adjusted to incorporate the nuclear data knowledge available in the integral benchmarks.

The results presented in this chapter will have an impact on the field of evaluation of nuclear reactions in the resolved resonance region. That impact will further propagate to the working communities that use the evaluated nuclear data. One such user community in particular is nuclear criticality safety. Nuclear criticality safety analyses the safe design and operation of nuclear material storage and transportation. This includes spent fuel pools and dry storage facilities at operating nuclear power plants, nuclear fuel processing facilities as well as nuclear material transportation and disposal. The law requires that the designers of these systems be able to show that they are below the set safety margins 95% of the time with 95% confidence. This means that the designs need to be conservative, not to expose the public to any unnecessary danger. On the other hand, it is a multi-million dollar business, where unjustified over-conservative design carries substantial costs. This community must rely heavily on an accurate knowledge of the nuclear data as well as an honest representation of the true state of knowledge of that nuclear data. The work in this dissertation on the accurate representation of the angular distribution of scattering and its impact
on criticality not only implies a needed re-analysis of how accurately the angular distributions are known for other materials, it also brings up another safety concern; shielding calculations. Shielding calculations rely heavily on the knowledge of scattering distributions to calculate the expected dose at a point in space, in particular, a radiation worker. Without an accurate representation of the angular distribution in radiation transport calculations, the radiation worker may be exposed to a larger dose than predicted by computer simulations. On the other side, the newly developed coupling methodology of the differential and integral data analysis can be used for any isotope to better understand how well the nuclear data is known for that isotope. Using the coupling methodology developed here, the evaluator will be able to report resolved resonance region evaluations with better understanding of the uncertainty of reported cross sections. Such adjustment may show that certain storage or transportation systems have been designed over-conservatively, in the case that the covariance data decreases as a result of the integral data feedback. Even small changes can result in large financial gains and reduced land and material footprint of the nuclear industry. On the other hand, in the case that the covariance data increases as a result of the integral data feedback, it will be understood that according to the law the accident risk for current storage or transportation systems was too large and a more conservative design must be adopted.
Chapter 5

Conclusions

This dissertation describes four significant contributions made to the field of resolved resonance region evaluation.

1. Experimental measurements of the cross section as a function of neutron energy in the thermal energy region for improved understanding of the negative-energy, external resonances and more realistic shape and uncertainty of the thermal cross section.

2. Evaluation of both the total and the capture cross section in order to properly determine the capture to scattering ratio.

3. Producing a high fidelity model for angular distributions that will be self-consistent with the reported resonance parameters and developing the mathematical framework for temperature broadening of these angular distributions. The importance of both of these contributions has been evaluated on criticality safety benchmarks and produced significant changes in $k_{eff}$.

4. Coupling of the differential and integral data analysis via direct feedback through the resonance parameters. The newly developed methodology allows for a systematic adjustment of all of the reactions, including the differential reactions with respect to angle and energy, based on suggested cross section changes from integral experiments while maintaining a proper fit of the cross section
experimental data. In the new methodology, the covariance of the resonance parameters can be updated to reflect the true state of knowledge based on more information than just cross section measurement experiments.

A new copper resolved resonance evaluation is vital to the safe operation of the advance fuel cycle. Copper is used as a constituent structure material in many fission applications. Of particular importance to the advance fuel cycle is the use of copper in spent fuel storage and transportation. Besides its current and future uses in the advance fuel cycle on the fission side, copper is also used in the field of fusion research. Lastly, copper is also part of the s-process studied by astrophysics trying to understand stellar evolution. The current standard of the resolved resonance region evaluation of the two copper isotopes in ENDF/B-VII.1 has been found to be inadequate and a new evaluation for the two isotopes of copper is wanting. This Ph.D. research makes several developments in the field of resolved resonance region evaluation using as backdrop the work on producing a new evaluation for the two isotopes of copper, $^{63,65}\text{Cu}$.

The first part of this research involved setting up and measuring new experimental data for the two isotopes of copper, $^{63,65}\text{Cu}$. Experimental measurements recorded the total cross section of two isotopic samples of copper between 0.01 eV and 0.1 eV, the thermal energy range. The specific purpose of these experiments was to obtain experimentally measured cross section versus energy and quantify the uncertainty of the cross section in an energy region where no other experimental data was available. The new experimental data allowed for a treatment of the uncertainties in the thermal energy region that reflected the true state of knowledge rather than an assumption based on theoretical models, as was done in the past. Furthermore, the fact the the experimental measurements provided the cross section as a function of energy, allowed a more accurate fitting of the negative external levels.

The over arching goal of developing a new evaluation of the resolved resonance region of copper was to remove doubt from the quality of the current standard. However, along the process of producing a new evaluation, an understanding was gained of multiple problems in the traditional evaluation approach. First, it was
shown that for non-fissile isotopes, evaluation of only total cross section experimental data cannot give the correct capture to scattering ratio. Next, it was found that an average treatment of the scattering angular distributions results in self*-inconsistent nuclear data. Finally, it was understood that one of the largest problems in evaluating differential experimental data for capture or scattering comes in the form of systematic uncertainties, such as normalization and background.

The new evaluations extended the resolved resonance region from 99 keV to 300 keV. Upon completion of the evaluation, it was shown that 300 keV was the upper bound in energy of the importance of self-shielding in criticality safety applications. A new automated routine to help establish the initial distribution of resonance quantum angular momentum was developed and applied to the new evaluation. Experimental capture data was evaluated for copper for the first time. Obtaining the correct capture to scattering ratio for the entire energy region from 1e-5 eV to 300 keV has obvious implications for neutronics calculations of models involving copper. The average treatment of the angular distribution of scattering in the current evaluations for copper was replaced by a high fidelity model of the angular distributions. The high fidelity model gives the angular distribution on a tight energy grid and includes the naturally occurring resonances in the scattering angular distribution. The ability to correctly represent the scattering angular distribution lies principally in identifying the quantum angular momentum of each resonance correctly. It was further shown that the impact of the high fidelity treatment of the angular distribution of scattering has a great effect on the criticality of small systems particularly where the material in question is used as a reflector. Lastly, for the evaluation part, a mathematical formalism was developed to allow for the temperature broadening of the angular distribution directly from the unbroadened distribution and the unbroadened angle-integrated cross section. In fact, as discussed in Section 3.2.4, temperature broadening is possible from any initial temperature, $T_0$ to any higher temperature. The initial temperature does not need to be 0 K. The temperature broadening methodology of angular distributions developed in this work was tested against angular distributions reconstructed from traditionally broadened differential cross sections and found to
match within numerical error. Furthermore, it was shown for the two isotopes of copper that temperature broadening the angular distribution of elastic scattering does not only better represent the behavior of the cross section in a realistic way, it also has an impact on the computed $k_{eff}$ of integral criticality safety benchmarks. In Section 4.3, it was shown that in a certain experiment (where a large mass of copper was used as a reflector in a small critical experiment with an impactful neutron spectrum) a difference of as much as 105.6 pcm has been observed. Besides such a drastic effect on one of the benchmarks, temperature broadening of the angular distributions of elastic scattering proved to provide statistically better results across all four of the intermediate-spectrum Zeus cases.

The benchmarking of the new evaluation prior to application of the new feedback loop from integral experiments showed statistical improvement in several of the outlying benchmarks. There was an overall statistical improvement of $320 \pm 225$ pcm for the 23 benchmarks. The four Zeus benchmarks showed a combined improvement of $202 \pm 96$ pcm.

In the final part of this research a new methodology for extracting the valuable nuclear data information that is available in the integral benchmarks was developed. The new methodology proposes a way of integrating the additional available information in the integral data into the resolved resonance region evaluation and interpreting that information in such a way as to consistently change the resonance parameters and update the covariance data. This research showed that it was possible to update the state of knowledge, the covariance data, by systematically adjusting the resonance parameters in such a way as to reflect suggested cross section changes based on information from critical experiments with in the uncertainty bounds of the experimental data.

The goal of this work was not to determine how to use sensitivity/uncertainty analysis codes such as TSURFER to improve cross section evaluation. Such work was done in validating TSURFER by its authors. The key to this Ph.D. research was to show that it is possible to couple the information output from TSURFER all the way back to the fundamental resonance parameters not just to multi-group cross
sections. Coupling back to the resonance parameters allows all of the reaction cross sections to be updated simultaneously, including the multi-dimensional cross sections and covariance data.

For the two new evaluations of copper developed in this work, TSURFER suggested a maximum change in the cross sections of 0.3%. This is interpreted as an indication of good quality of the new resolved resonance region evaluations based only on differential experimental data. The magnitude of the suggested cross section change was not enough to show statistically improved results in the integral benchmark calculations based on the updated resonance evaluations. However, it was clearly demonstrated that the coupling of the integral data feedback to the resonance parameters results in the necessary changes in the reconstructed cross sections and systematic, self-consistent changes in the multi-dimensional nuclear data. Further, it was shown that such suggested cross section changes based on integral data result in smaller associated covariance data.

The newly developed coupling methodology is proposed to be used as another tool in the evaluators tool box. The development of the systematic procedure, means that less emphasis will be put on the evaluator's expertise and judgment of how to interpret the limited, non-quantitative, feedback traditionally received from evaluation benchmarking on integral experiment computer models.

The new developments for resolved resonance region evaluation made in this research will have a significant impact on this field of science. This research has highlighted several gaps in the current practices for the resolved resonance region evaluation and has developed new methodologies to fill in those gaps. In particular, in order to avoid using an approximation for the thermal energy region, it has been described how simple experimental measurements of the neutron cross section in the thermal energy region can be used to determine the resonance parameters of the negative energy external resonances. Such experimental measurements can be made for almost any isotope and would have an impact on the shape and uncertainty of the cross section in the thermal energy region. Further, it was demonstrated that no evaluation can be complete without evaluating both the transmission and the cap-

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ture experimental data. Existing evaluations done on only transmission experimental data should be questioned on the accuracy of the capture to scattering ratio. A big contribution to the field of resolved resonance region evaluation from this research has been the demonstration of the need of high-fidelity, self-consistent angular distributions for scattering. The findings of this work, bring into question the validity of all of the angular distributions for resolved resonance region reactions in nuclear data repositories. The concluding paragraph of this chapter discusses such a possibility as future work stemming from this original research. The mathematical framework for temperature broadening of the angular distributions independent from the differential cross section has been developed and its impact on criticality safety calculations demonstrated. This technique can be implemented in nuclear data processing codes to temperature broaden the angular distributions along with angle integrated cross sections. Furthermore, the newly developed temperature broadening technique does not require the knowledge of resonance parameters and can be applied to any isotope with angular distributions and angle integrated cross sections available. No equivalent currently exists in any of the processing codes. Finally, a methodology has been developed to couple the nuclear data information available in the integral experiments to a systematic updating of the resonance parameters. This practice allows for self-consistent changes in all of the reactions as well as an updating of the reported covariance data to better reflect the true state of knowledge of the resonance parameters. This new methodology can now be applied to new and existing evaluations to use more data than was previously available only in differential cross section measurements. Particularly, this new methodology can be applied to many of the isotopes that have questionable quality covariance data, to evaluate the true state of knowledge based on the immense nuclear data information contained in integral benchmarks.

Future work that could build of this Ph.D. project might want to explore a derivation of analytic expressions starting from the reduced R-matrix theory and how the resonance parameters should be varied to reflect the necessary cross section changes. This is already done indirectly in this work through the SAMMY code. However,
certain advantage could be found in doing what SAMMY does through a chi-squared fitting directly through analytical expressions.

There is still much more work to be done in traditional nuclear data. Even though, there has been much progress made in decreasing the discrepancy in the Zeus benchmarks by providing a new resolved resonance region evaluation, the problem is not entirely solved. The key to the solution could lie in the resolved resonance region evaluations of the other major materials ($^{235}$U, $^{12}$C). Perhaps, the angular distribution of $^{12}$C as a function of energy is the culprit. Finally, the high energy evaluation of any of the isotopes, including copper, could be the right answer.

A different direction that has been highlighted by this research is the importance of the angular distributions. The angular distributions reported in the resolved resonance region evaluations of other isotopes should be reconsidered. An evaluation will have to be made of the reliability of the distribution of quantum angular momentum throughout the resonance region to ensure that the differential scattering cross sections can be reconstructed correctly. After this, high fidelity angular distributions can be calculated from the differential scattering cross sections and reported along with the resonance parameters to nuclear data repositories. The studies of the angular distribution is not limited to only the elastic scattering cross section nor is it, in fact, limited to the resolved resonance region. The inelastic scattering channel for the two isotopes of copper studied in this work opens up well beyond the new upper boundary of the resolved resonance region. However, the author hopes to, in the near future, study the effects of the angular distribution and its temperature broadening for both discrete inelastic and continuous inelastic scattering reactions. Further, there are possibilities to expand the study of angular distributions to the unresolved resonance region. With the importance of angular distributions highlighted here, the possibilities are practically endless; sensitivities and covariance data can be explored for angular distributions. There is already provisions made in the ENDF6 format, although it is hardly ever used, for reporting the covariance of the angular distributions. Finally, the newly developed coupling methodology of differential and integral data analysis could also be applied based on required differential cross sec-
tion changes (changes in the angular distributions) once sensitivity and uncertainty analysis of angular distributions is developed that far.
Appendix A

Detailed Photographs of the MITR neutron-TOF experiment
Figure A-1: A photograph of the MITR neutron-TOF experimental set up.
Figure A-2: A photograph of the MITR neutron-TOF BF$_3$ neutron detector. The detector is behind the white polyethylene neutron collimator.
Figure A-3: A photograph of the MITR neutron-TOF cadmium neutron chopper.
Appendix B

Radiate Capture Cross Section Measurements in the Thermal Energy Region at the neutron-TOF Experiment at the MITR

B.1 Introduction

The purpose of the study was to create an experimental set-up and show its capability to measure $^{63,65}$Cu thermal neutron capture cross sections. Currently, there is no experimental capture cross section data versus energy in the thermal energy region for either isotope of copper in the EXFOR database. [32] Such experimental data would compliment the total thermal cross section measurements carried out at the same experimental facility. Thermal capture cross section data spanning a neutron energy region from 0.01 eV to 0.1 eV would uniquely define all of the reaction cross sections for the two isotopes of copper in the thermal energy region. This data would also aid in determining the parameters of the negative-energy external resonances for the new resonance evaluations and reduce the associated uncertainties. Preliminary tests with $^{63,65}$Cu and $^{113}$Cd (used as a reference case) samples demonstrated that the
new experimental set up can detect the characteristic gamma rays produced at levels higher than background. However, upon careful determination of the neutron beam flux and evaluation of the efficiency of the experimental set up, it was determined that a cross section measurement at several neutron energies and with good statistics is impossible in a reasonable amount of time.

What follows is a description of the experimental efforts in this direction for archival purposes.

B.2 Background

The developed experimental set-up was tested to show its capability to measure the characteristic gamma rays of the two copper samples. The reactions for the radiative neutron capture of $^{63}\text{Cu}$ and $^{65}\text{Cu}$ are shown below:

egin{align*}
^{63}\text{Cu}(n,\gamma)^{64}\text{Cu} & \quad \text{(B.1)} \\
^{65}\text{Cu}(n,\gamma)^{66}\text{Cu} & \quad \text{(B.2)}
\end{align*}

Table B.1 gives the values of the major characteristic gamma rays of each sample and their associated probabilities per captured neutron. There are many characteristic gamma rays that are released from the above described reactions. The gamma ray energies listed in Table B.1 are the ones that appear in the detector energy domain and at the highest probability for each copper isotope.

Table B.1: Characteristic $\gamma$ rays of the $^{63}\text{Cu}(n,\gamma)^{64}\text{Cu}$ and $^{65}\text{Cu}(n,\gamma)^{66}\text{Cu}$ reactions

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Energy (keV)</th>
<th>Intensity Max (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{63}\text{Cu}$</td>
<td>278.24</td>
<td>72.51</td>
</tr>
<tr>
<td></td>
<td>159.28</td>
<td>45.32</td>
</tr>
<tr>
<td></td>
<td>608.75</td>
<td>23.56</td>
</tr>
<tr>
<td>$^{65}\text{Cu}$</td>
<td>186.01</td>
<td>100.00</td>
</tr>
<tr>
<td></td>
<td>385.78</td>
<td>46.34</td>
</tr>
<tr>
<td></td>
<td>543.85</td>
<td>10.22</td>
</tr>
</tbody>
</table>
The peculiar way in which the intensity of the characteristic gamma rays is provided stems from the Evaluated Nuclear Structure Data File (ENSDF) [2] which defines the intensity of each gamma ray relative to the intensity of the most probable gamma ray for the reaction. The reason for this format is that for some isotopes (\(^{65}\)Cu included) the absolute intensity of the gamma rays is not known per incident neutron. Only the intensity relative each other has been measured. For \(^{63}\)Cu the maximum intensity is \(33.10 \pm 0.60\) per neutron captured.

In order to deduce the radiative capture cross sections of \(^{63,65}\)Cu one needs to be able to discriminate between gamma rays of different intensities. Then, the identified characteristic gamma rays can be counted and the number of \((n, \gamma)\) reactions occurring in each sample can be calculated. At first it appears as if in order to calculate the number of \((n, \gamma)\) reactions, the experimenters must have good information about the efficiency of their gamma detector, the detector geometry and the multiple scattering and self-shielding of the sample. However, the first two of these troubles can be eliminated simply by doing a measurement relative to a well known capture cross section standard, for example, gold. The different response of the gamma ray detector to gamma rays of different energies is well known by the manufacture and can be corrected for. The other effects can be taken into account in the data analysis. Doing the measurement as a relative measurement against a well known standard also has the advantage of not needing to know the neutron beam flux characteristics. The downfall of this method is that large correlations are introduced between cross sections of the measured isotope and the standard isotope.

**B.3 Methods**

**B.3.1 Experimental Set-up**

The energy discrimination used in the radiative capture set-up utilized the same cadmium neutron chopper wheel, see Figure A-3, as the transmission measurement. Therefore the same resolution function characteristics existed for this experiment as
for the transmission experiment described in Section 3.1 except the flight path which had been extended to 185 cm in designing the new experiment.

In the experimental design, it was proposed that a multi-channel analyzer be connected to the Canberra High Purity Germanium Detector (HPGe).\footnote{A Canberra Standard Electrode Coaxial Germanium Detector was used for the gamma ray detection.} This way, the neutron time of flight; from the time the packet of neutrons is released by the cadmium chopper wheel to the time the neutrons interact in the sample and produce a gamma ray, can be measured and recorded. The neutron velocity and energy can be calculated with this time of flight value and the known flight distance. Since, the Canberra HPGe detector measures the incident gamma ray energy, a full gamma ray energy spectrum would be available for each neutron energy (time of flight). In the post-processing of the data, it would be possible to associate a measurement of the characteristic gamma ray of each isotope with a radiate capture event that occurred at a specific neutron energy. Therefore, a full reconstruction of the thermal capture cross section should be possible.

In order to measure statistically-significant gamma peaks, background counts must be minimized. For this reason, the HPGe detector was housed in 10 cm thick lead-brick shielding (for gamma background) and 2.5 cm Borated polyethine shielding (for neutron background). A window opening in the shielding box facing the sample allowed for the sample-generated gammas to enter the detector. The sample was located 6 cm away from the detector. A schematic drawing of the experimental set up is given in Figure B-1.

**B.3.2 Experimental Procedures**

Each test followed a similar set of procedures.

- First, the HPGe detector's energy spectrum would be calibrated within 0.1 keV using three characteristic gamma energy peaks from two well known test sources; \(^{60}\text{Co}\) and \(^{137}\text{Cs}\). This step gives reliability to the energy values of the sample emitted gammas.
Figure B-1: Modification of the transmission experimental set up (inside the dotted lines) for the radiative capture measurements.

- Before each measurement, a sample-out measurement was made of the local background in the experimental facility. The sample-out counts could then be subtracted from the sample-in counts as a means of background correction.

- To interrogate a sample, it was aligned with the beam line and detector shielding window and held in place with a clamp. The chopper wheel was either lifted out of the beam line for a simple proof of concept experiment or turned on to spin and collect energy discrimination data for a cross section measurement versus neutron energy experiment.

- The neutron beam shutter was opened to let the neutrons out of the port. The HPGe detector measured the gammas produced by the sample and saved the data for post-processing.

The isotope $^{113}\text{Cd}$ was also used in the diagnostics experiments on the radiative capture set up. The isotope $^{113}\text{Cd}$ has a neutron capture cross section that is on the order of $10^3$ greater than that of either of the copper isotopes. An available isotopic sample of $^{113}\text{Cd}$ was used to obtain better statistics in shorter run times. The particular need for the $^{113}\text{Cd}$ sample arose because the cadmium chopper wheel cuts down approximately 97% of the neutron beam flux, so in the preliminary tests $^{113}\text{Cd}$ sample was used to generate a satisfactory number of counts.
B.4 Preliminary Results

The objective of this proof-of-concept study was to test a set-up that could later be used to gather data to measure the thermal capture cross section of the two copper isotopes. Table B.2 shows a summary of the completed tests.

B.5 Discussion

A sample output of the HPGe gamma ray detector is given in Figure B-2 for the beam-on background measurement. The 511 keV annihilation gamma ray line is clearly visible and many other characteristic gamma lines can be identified.

The $^{113}\text{Cd}$ test results confirmed that the electronic time discrimination and HPGe detector set-up were operational. The two copper tests showed that the current assembly is capable of producing a significant count rate above background for the copper characteristic gamma peaks, see Figure B-3. The two $^{63}\text{Cu}$ characteristic gamma rays are distinctly visible at 159 keV and 278 keV. The $^{65}\text{Cu}$ line clearly shows the 186 keV characteristic gamma ray line. However, these experiments were made without any neutron energy discrimination.

After a study of the MIT Reactor beam port used for this experiment, it was determined that the thermal neutron flux is only about 19,000 $\text{neutrons/cm}^2\text{s}$. A simple back-of-the-envelope calculation proves that with such a neutron flux, measurement of the thermal neutron capture cross section for the two isotopes of copper.

### Table B.2: Results of Set-up Diagnostics Experiments

<table>
<thead>
<tr>
<th>Beam</th>
<th>Sample</th>
<th>Chopper</th>
<th>Gamma Energy (keV)</th>
<th>Count Rate per Hour</th>
<th>Reason</th>
</tr>
</thead>
<tbody>
<tr>
<td>Off</td>
<td>None</td>
<td>Off</td>
<td></td>
<td></td>
<td>Reactor background</td>
</tr>
<tr>
<td>On</td>
<td>None</td>
<td>Off</td>
<td></td>
<td></td>
<td>Beam background</td>
</tr>
<tr>
<td>On</td>
<td>$^{113}\text{Cd}$</td>
<td>Off</td>
<td>558.5</td>
<td>1067</td>
<td>Energy discrimination</td>
</tr>
<tr>
<td>On</td>
<td>$^{113}\text{Cd}$</td>
<td>On</td>
<td>558.5</td>
<td>35</td>
<td>Energy discrimination</td>
</tr>
<tr>
<td>On</td>
<td>$^{63}\text{Cu}$</td>
<td>Off</td>
<td>278</td>
<td>1116</td>
<td>$^{63}\text{Cu}$ gamma detection</td>
</tr>
<tr>
<td>On</td>
<td>$^{63}\text{Cu}$</td>
<td>Off</td>
<td>159</td>
<td>396</td>
<td>$^{63}\text{Cu}$ gamma detection</td>
</tr>
<tr>
<td>On</td>
<td>$^{65}\text{Cu}$</td>
<td>Off</td>
<td>186</td>
<td>180</td>
<td>$^{65}\text{Cu}$ gamma detection</td>
</tr>
</tbody>
</table>
Figure B-2: Output of the HPGe gamma ray detector for the background test run. The bottom plot shows the entire energy domain of the detector with the number of counts on the vertical axis and the top plot is the zoomed in look at the energy region selected within the box.

Figure B-3: Gamma ray spectra plotted for the $^{63}$Cu, $^{65}$Cu and background.
is impossible with any reasonable statistics. Even under the most extreme assumptions of 100% of the beam interacting in the sample and 100% gamma ray escape probability from within the sample, the required run time for good statistics is on the order of weeks. Such a run time is impossible at a university experimental reactor.

B.6 Conclusions

An experimental facility was created and tested at the MIT Reactor to measure the thermal neutron capture cross section of $^{63,65}$Cu. The experimental set up implements a Canberra HPGe gamma ray detector to select characteristic gamma rays and the neutron time-of-flight technique for neutron energy discrimination. The facility has been shown to be able to measure the characteristic gammas of both isotopes of copper at a rate above the background level and neutron energy discrimination for the measurement of the neutron capture cross section has been shown viable on the $^{113}$Cd sample. However, the thermal neutron flux in the beam has been determined severely insufficient for neutron cross section measurements with acceptable statistics.
Appendix C

Selected Integral Benchmark Experiments

All of the material presented in this section is compiled from the ICSBEP Handbook [5].

C.1 HMF072

Zeus: Fast-Spectrum Critical Assemblies with an Iron-HEU Core Surrounded by a Copper Reflector

The Zeus experiments were assembled on the general-purpose Comet vertical assembly machine. The assemblies consist of a cylindrical core region containing interspersed plates of HEU metal and carbon steel that are surrounded on all sides by a metallic copper reflector. The assembly is divided into two portions. The upper part of the reflector, which includes the upper, corner, and side reflectors, rests on a stationary aluminum support plate (Top Plate) attached to the Comet machine. The upper segment of the core rests on a thin, square stainless steel plate, which is supported by copper corner reflectors. The remainder of the core and the lower reflector are seated on a circular aluminum platen adapter plate connected to the vertical drive (ram) of the assembly machine. The lower core plates and the lower reflector are held in position by a central, hollow aluminum alignment tube. The
experiment is assembled by raising the lower portion into the reflector until it fully closes to the steel diaphragm that supports the upper segment of the core. There are no other control, safety, or shim rods inside the assembly.

A photograph of the Zeus assembly on the Comet machine is shown in Figure C-1. The bottom copper reflector and two graphite moderator plates can be seen resting on the platen adapter plate. The central alignment tube also is clearly visible.

Figure C-2 shows a schematic view inside the Zeus experimental set up. The major components outlined in the diagram are the \textit{SR}, \textit{UR}, and \textit{LR}, which stand for \textit{side}, upper, and lower reflector and the fuel plates are shown by the gray color in the middle of the diagram.

\section*{C.2 HMI006}

\textbf{The Initial Set of Zeus Experiments: Intermediate-Spectrum Critical Assemblies With a Graphite-HEU Core Surrounded by a Copper Reflector}

The Zeus experiments were assembled on the general-purpose Comet vertical assembly machine. The assemblies consisted of a cylindrical core region containing interspersed plates of HEU metal and graphite that were surrounded on all sides by metallic copper reflectors.

The basic building block of the Zeus cores is referred to as a unit. A unit consists of an inner HEU disk and an outer HEU ring that fit snugly together, along with an equal number of graphite plates above and below the HEU. Zeus experiments 1, 2, 3, and 4 contained 8, 6, 4, and 2 graphite plates per unit, respectively. The assembly is divided into two portions. The top, corner, and side reflectors rest on a stationary aluminum support plate attached to the Comet machine. The top and bottom segments of the core each contain an integral, although different, number of units. The top segment of the core rests on a thin, square stainless steel plate, called the diaphragm, which is supported by copper corner reflectors. The bottom segment of the core sits on top of the bottom reflector. The bottom reflector, in turn, is seated on a circular aluminum platen adapter plate, which is connected to the platen.
Figure C-1: The Zeus assembly mounted on the Comet machine.
Figure C-2: Vertical slice through the Zeus assembly
of the vertical drive (ram) of the assembly machine. The lower core plates and the bottom reflector are held in position by a central, hollow aluminum alignment tube. The experiment is assembled by raising the bottom portion of the assembly into the corner reflectors until it fully closes against the steel diaphragm that supports the top segment of the core. There are no other control, safety, or shim rods inside the assembly.

A photograph of the Zeus assembly on the Comet machine is shown in Figure C-1. The bottom copper reflector and two graphite plates can be seen resting on the platen adapter plate. The central alignment tube also is clearly visible.

Figure C-2 shows a schematic view inside the Zeus experimental set up. The major components outlined in the diagram are the $SR, UR,$ and $LR,$ which stand for side, upper, and lower reflector and the fuel is shown by the gray color in the middle of the diagram. The difference between the four HMI006 cases would be reflected in Figure C-2 by different vertical thicknesses of the fuel region. For example, for case 1, where 8 graphite plates per HEU plate were used, the upper reflector would align with the top of the side reflector.

The neutron spectra for the four cases of HMI006 are plotted in Figure C-3. The neutron spectrum gets harder with increasing case number. This is effect is achieved by varying the carbon to uranium ratio ($C/U$) from approximately 50 to 13 going across the four cases.

C.3 LCT009

Water-Moderated Rectangular Clusters of $U(4.31)O_2$ Fuel Rods (2.54-cm Pitch) Separated by Steel, Boral, Copper, Cadmium, Aluminum, or Zircaloy-4 Plates

A series of critical-approach experiments with clusters of 36-inch-long aluminum-clad $U(4.31)O_2$ fuel rods in a large water-filled tank was performed. The selected cases used water-reflected experiments with 3 rectangular clusters of 2.54-cm-pitched rods. Two absorber plates separated the two outer clusters from the center one. The
plates were made of copper or copper-copper with 1% cadmium. Six cases were used in this work.

Figure C-4 shows a photograph of the unloaded experimental tank. The lattice structural plates are clearly distinguishable for three separate fuel clusters. The solid plates above the lattice support structure are actually safety blade guides. Whereas, the copper separation plates were positioned on either side of the center fuel cluster at a measured distance reported in Table C.1. Figure C-5 is a schematic of the setup of a different case from the same benchmark configuration. The only difference in Figure C-5 from the cases used in this work, is that the borated steel plates were replaced by copper plates.

C.4 LCT012

Water-Moderated Rectangular Clusters of U(2.35)O₂ Fuel, Roads (1.684-cm Pitch) Separated by Steel, Boral, Boroflex, Cadmium, or Copper Plates
Figure C-4: Experiment tank, lattice plates for 3 clusters, and control/safety blades.

Figure C-5: Typical critical configuration for LCT009. For the cases selected for this work, the borated steel plates were replaced by copper plates.
(Gadolinium Water Impurity)

A series of critical-approach experiments with clusters of 36-inch-long aluminum-clad U(2.35)O2 fuel rods in a large water-filled tank was performed. The selected cases were water-reflected experiments performed with 3 rectangular clusters of 1.684-cm-pitched rods with neutron-absorber plates between clusters with a reported small Gd impurity in the water moderator-reflector. The absorber plates were copper, or copper with 1% cadmium. Two cases were used in this work.

Figure C-4 shows a photograph of the unloaded experimental tank. The lattice structural plates are clearly distinguishable for three separate fuel clusters. The solid plates above the lattice support structure are actually safety blade guides. Whereas, the copper separation plates were positioned on either side of the center fuel cluster. Figure C-6 is a schematic of the setup of a different case from the same benchmark configuration. The only difference in Figure C-6 from the cases used in this work, is that the steel plates were replaced by copper plates. Table C.2 gives some dimensional data for the two selected cases.
C.5 LCT013

Water-Moderated Rectangular Clusters of U(2.35)O₂ Fuel Roads (1.684-cm Pitch) Separated by Steel, Boral, Boroflex, Cadmium, or Copper Plates with Steel Reflective Walls

A series of critical-approach experiments with clusters of 36-inch-long aluminum-clad U(4.31)O₂ fuel rods in a large water-filled tank was performed. The selected cases were water-reflected experiments, performed with 3 rectangular clusters of 1.892-cm-pitch rods with absorber plates between clusters and steel walls on either side of the line of fuel clusters. The two types of absorber-plate were copper and copper with 1% cadmium. The experimenters found that the effectiveness of the neutron absorber plates to reduce the critical separation between fuel clusters is reduced slightly by the presence of the steel reflecting walls. Two cases were used in this work.

Figure C-4 shows a photograph of the unloaded experimental tank. The lattice structural plates are clearly distinguishable for three separate fuel clusters. The solid plates above the lattice support structure are actually safety blade guides. Whereas, the copper separation plates were positioned on either side of the center fuel cluster. The stainless steel reflecting walls are not shown in the photo of Figure C-4.
Figure C-7 is a schematic of the setup of a different case from the same benchmark configuration. The only difference in Figure C-7 from the cases used in this work, is that the steel plates were replaced by copper plates. Figure C-7 shows the location and size of the stainless steel reflector walls relative to the fuel clusters and separation plates. Table C.3 gives some dimensional data for the two selected cases.

C.6 LCT016

Water-Moderated Rectangular Clusters of U(2.35)O₂ Fuel Rods (2.032-cm Pitch) Separated by Steel, Boral, Copper, Cadmium, Aluminum, or Zircaloy-4 Plates

A series of critical approach experiments with clusters of 36-inch-long aluminum-clad U(2.35)O₂ fuel rods in a large water-filled tank was performed. The selected cases were water-reflected experiments with 3 rectangular clusters of 2.032-cm-pitched rods. Two absorber plates separated the two outer clusters from the center one. The plates were copper or copper with 1% cadmium. Six cases were used in this work.

Figure C-4 shows a photograph of the unloaded experimental tank. The lattice structural plates are clearly distinguishable for three separate fuel clusters. The solid plates above the lattice support structure are actually safety blade guides. Whereas, the copper separation plates were positioned on either side of the center fuel cluster at a measured distance reported in Table C.1. Figure C-8 is a schematic of the setup of a different case from the same benchmark configuration. The only difference in Figure C-8 from the cases used in this work, is that the steel plates were replaced by copper plates.

<table>
<thead>
<tr>
<th>Case</th>
<th>Material</th>
<th>Thickness (mm)</th>
<th>Separation of Fuel Clusters (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Copper</td>
<td>3.37 ± 0.08</td>
<td>134.7 ± 0.4</td>
</tr>
<tr>
<td>7</td>
<td>Copper-Cadmium</td>
<td>3.57 ± 0.08</td>
<td>105.7 ± 0.2</td>
</tr>
</tbody>
</table>
Figure C-7: Typical critical configuration for LCT013. For the cases selected for this work, the steel plates were replaced by copper plates.

Figure C-8: Typical critical configuration for LCT016. For the cases selected for this work, the steel plates were replaced by copper plates.
Table C.4: U(2.35)O₂ Fuel-Rod Cluster Critical Configures with Copper Plates

<table>
<thead>
<tr>
<th>Case</th>
<th>Cluster Dimensions (number of rods)</th>
<th>Cd Content (wt.%)</th>
<th>Thickness (mm)</th>
<th>Distance to Center of Fuel Cluster (mm)</th>
<th>Separation of Fuel Clusters (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>20 x 16</td>
<td>0.0</td>
<td>6.46 ± 0.08</td>
<td>6.45 ± 0.06</td>
<td>66.2 ± 0.2</td>
</tr>
<tr>
<td>16</td>
<td>20 x 16</td>
<td>0.0</td>
<td>6.46 ± 0.08</td>
<td>27.32 ± 0.50</td>
<td>77.2 ± 0.6</td>
</tr>
<tr>
<td>17</td>
<td>20 x 16</td>
<td>0.0</td>
<td>6.46 ± 0.08</td>
<td>44.42 ± 0.60</td>
<td>75.1 ± 0.2</td>
</tr>
<tr>
<td>18</td>
<td>20 x 15 (center) 24 x 15 (outer)</td>
<td>0.0</td>
<td>3.37 ± 0.08</td>
<td>6.45 ± 0.06</td>
<td>68.8 ± 0.5</td>
</tr>
<tr>
<td>19</td>
<td>20 x 15 (center) 24 x 15 (outer)</td>
<td>0.0</td>
<td>3.37 ± 0.08</td>
<td>40.42 ± 0.70</td>
<td>70.0 ± 0.4</td>
</tr>
<tr>
<td>20</td>
<td>20 x 15 (center) 24 x 15 (outer)</td>
<td>0.989</td>
<td>3.57 ± 0.08</td>
<td>6.45 ± 0.06</td>
<td>51.5 ± 0.6</td>
</tr>
</tbody>
</table>

The neutron spectra for two cases of LCT016 are plotted in Figure C-9. Case 32, shown in Figure C-9 is irrelevant to this work, as that case did not have any copper content. However, the spectrum for case 20, is relevant and a good representation of the shape of the spectrum for most of the LCT benchmarks used in this work.

C.7 LCT042

Water-Moderated Rectangular Clusters of U(4.31)O₂ Fuel, Roads (1.892-cm Pitch) Separated by Steel, Boral, Boroflex, Cadmium, or Copper Plates with Steel Reflective Walls

A series of critical approach experiments with clusters of 36-inch-long aluminum-clad U(2.35)O₂ fuel rods in a large water-filled tank was performed. The selected cases were water-reflected experiments with 3 rectangular clusters of 1.684-cm-pitched rods with absorber plates between clusters and steel walls on either side of the line of fuel clusters. The absorber-plate types were copper and copper with 1% cadmium. Two cases were used in this work.

Figure C-4 shows a photograph of the unloaded experimental tank. The lattice structural plates are clearly distinguishable for three separate fuel clusters. The solid plates above the lattice support structure are actually safety blade guides. Whereas, the copper separation plates were positioned on either side of the center fuel cluster.
Figure C-9: Neutron spectra for two cases of LCT016. The case 32 spectrum is not relevant for this work, only the case 20 spectrum is relevant.

The stainless steel reflecting walls are not shown in the photo of Figure C-4. Figure C-10 is a schematic of the setup of a different case from the same benchmark configuration. The only difference in Figure C-10 from the cases used in this work, is that the steel plates were replaced by copper plates. Table C.5 gives some dimensional data for the two selected cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>Material</th>
<th>Thickness (mm)</th>
<th>Separation of Fuel Clusters (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>copper</td>
<td>3.37 ± 0.08</td>
<td>77.9 ± 0.2</td>
</tr>
<tr>
<td>7</td>
<td>copper-cadmium</td>
<td>3.57 ± 0.08</td>
<td>54.3 ± 1.0</td>
</tr>
</tbody>
</table>
Figure C-10: Typical critical configuration for LCT042. For the cases selected for this work, the steel plates were replaced by copper plates.
Bibliography


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[29] Pereslavtsev, P. Private communication, August 2013.


