Monte Carlo Methods for Uncertainly Analysis Using the Bayesian R-Matrix Code SAMMY

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ABSTRACT

The Bayesian R-Matrix analysis code SAMMY is used for extracting resonance parameters from experimentally determined capture and transmission data. This procedure can sometimes produce resonance parameters with unrealistically low uncertainties due to a lack of experimental covariances included with the input data. During the recent analysis of the 5.47 eV resonance of ^{236}U at the Rensselaer Polytechnic Institute Gaerttner Linear Accelerator Center, a method was developed using Monte Carlo methods and SAMMY to extract accurate resonance parameters and uncertainties from a set of experimental neutron transmission data. All relevant input parameters, including sample data, background normalizations, time-of-flight parameters, and resolution function parameters, were sampled within their uncertainty probability distributions to obtain a complete set of transmission data and SAMMY input files for each Monte Carlo realization. Realizations were run until the standard deviation of the resulting resonance parameters, energy, neutron width, and radiation width, converged. The results were the resonance parameters and the associated uncertainties on those parameters. This computationally intensive but easy to perform method provided realistic uncertainties on the 5.47 eV ^{236}U resonance parameters by propagating all relevant input uncertainties through to the result.

KEYWORDS
SAMMY, Monte Carlo, Resonance Parameters, Uncertainty

1. INTRODUCTION

Experimental data were taken at the Gaerttner Linear Accelerator Center at Rensselaer Polytechnic Institute (RPI) in order to characterize the strong ^{236}U resonance at 5.47 eV [1]. A neutron transmission experiment was performed using the time-of-flight (TOF) method through three enriched ^{236}U sample thicknesses. Data were reduced to transmission, and these transmission data sets were analyzed using the Bayesian R-Matrix code SAMMY [2]. The code SAMMY is used for extracting useful resonance parameters from experimental transmission data. This method can sometimes provide unrealistically low uncertainties. One possible reason for these low uncertainties is the lack of adequate experimental

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covariance data provided to the code, as current data collection and reduction techniques do not provide full covariance parameters for experimental data [3]. Therefore, in order to obtain accurate resonance parameters and associated uncertainty information, a Monte Carlo method was employed to iteratively run the SAMMY code using experimental neutron transmission data. This method utilizes all the relevant input uncertainties for both the data reduction to transmission as well as the SAMMY analysis used to extract resonance parameters and determines the uncertainties on the resultant resonance parameters. This result is believed to be the best set of resonance parameters to fit the 5.47 eV ^{236}U resonance as well as the appropriate uncertainties on those values.

2. METHODS

2.1. Transmission

The transmission experiment utilized a high energy (~50 MeV) pulsed electron beam generated by the RPI linear accelerator to generate a pulsed neutron source. This neutron source was then collimated and passed through the samples of enriched ^{236}U. Data were collected using a 7.62 cm diameter by 0.3 cm thick ^{6}Li-glass scintillation detector for each of the three samples as well as an "open" position, without any material present in the neutron path. The transmission through each of the samples in its simplest form is the ratio of the counting rate collected with the sample in the beam to counts with the sample out of the beam:

$$Transmission = \frac{Count\ Rate_{Sample-IN}}{Count\ Rate_{Sample-OUT}}. \quad (1)$$

In order to approximate this ideal expression for the experiment the data collected must be corrected for such components as the neutron background rate, detector dead time, and differences between the sample-in and sample-out counting rates due to variations in the neutron beam intensity. Of these the most influential and difficult to determine is the time-dependent background hidden in the collected neutron spectra. The transmission in TOF channel *i*, T_i, is expressed as:

$$T_i = \frac{C_i^S - k^S B_i^S - B^S}{C_i^O - k^O B_i^O - B^O} \quad (2)$$

where C_i^S and C_i^O are the dead-time and neutron beam variance corrected sample and open beam count rates; B_i^S and B_i^O are the sample and open time-dependent backgrounds; k^S and k^O are normalization factors for the sample and open beam time-dependent backgrounds; and B^S and B^O are the steady-state background counting rates for sample and open measurements.

This experiment used fixed notches, present in all data collection, to obtain the time-dependent background at distinct energies. Local depressions caused by the black resonances, however, caused discrepancy as shown in Figure 1. The three points listed ^{115}In, ^{238}U, and ^{186}W are black notches (at the valley the transmission is less than 0.00) that cannot be connected by a realistic background function. Assuming the energy dependent background is a smooth function, there are no physical background shapes that could include all three points. Therefore, two bounding background functions were determined, the local notch (^{238}U) background and the distant notch (^{115}In, ^{186}W) background; the true background was assumed to lie between these limits and the difference between them contributes to the uncertainty in the transmission.

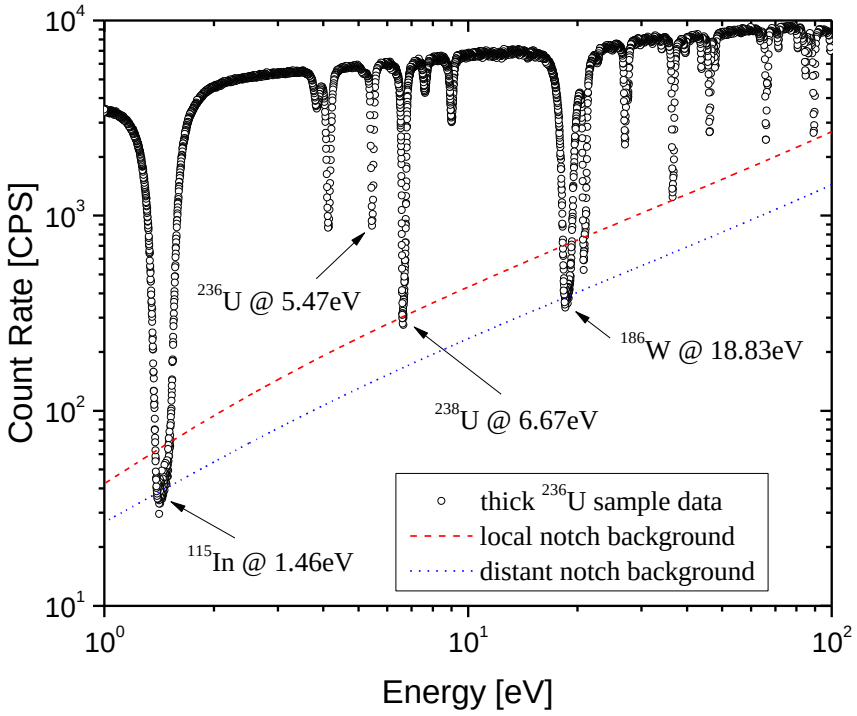

Figure 1. Experimental transmission data showing the bounding local and distant fixed notch background information.

The in-house computer code TRANS [4] was used to calculate the transmission from the experimental data using equation 2.

2.2. SAMMY Code

The experimental transmission data were input into the computer code SAMMY to extract resonance parameter information. SAMMY is a multi-level, multi-channel, R-Matrix code which employed a Reich-Moore approximation (other R-Matrix approximations could have been selected) and Bayesian statistical analysis to fit the shape of the experimental data using predicted resonance parameters. SAMMY can also be used to predict a number of other shape fitting experimental parameters, such as a normalization constant to the input data. The normalization accounts for an offset in the baseline transmission in the potential scattering region and may be used for uncertainties in sample composition.

Data input to the SAMMY code for this analysis included: experimental transmission and uncertainty, sample number densities, neutron flight path, effective Debye temperature, resolution function, initial guess of resonance parameter information (ENDF-7.1 [5] values), and isotopic information (channel spin, parity, abundance) for all components of the sample material. An important component influencing the fit to the transmission data is the energy resolution of the neutron production and collection system. The resolution function acts to broaden the data collected during the transmission experiment and must be included in the SAMMY calculation in order to match the experimental data. The resolution function, $R_T(E - E')$, represents the probability of detecting a neutron with energy E' at the same TOF as energy E. An ideal transmission, $T(E')$, at energy E' is convoluted by the resolution function to yield the experimental transmission, $T_{exp}(E)$, at energy E as follows:

$$T_{exp}(E) = \int_{E1}^{E2} R_T(E - E')T(E')dE'. \quad (3)$$

SAMMY takes this information and fits the experimental transmission, reporting the resulting resonance parameter information and a reduced chi-squared goodness of fit.

2.3. Monte Carlo Method

Monte Carlo is an established computational method in the nuclear community and has more recently been introduced into nuclear data uncertainty propagation. Koning and Rochman used Monte Carlo methods to propagate uncertainties in nuclear data to large scale nuclear reactor systems in order to obtain uncertainties on k_{eff} in criticality benchmarks [6]. This method, termed the Total Monte Carlo (TMC) method, repeatedly performed the same simulation while sampling from a pool of input parameters based on their individual uncertainties. TMC is computationally expensive but relatively easy to perform and is the basis for the methods used for uncertainty propagation here.

A program was written to generate SAMMY inputs (experimental data, experimental conditions, initial conditions) and run a complete SAMMY analysis on that set, store the results, and repeat using a new set of input parameters. An overview of the process is shown in Figure 2. Each simulation consisted of generating a complete set of transmission results using the TRANS code from the experimental data. Those parameters with the greatest effect on the transmission were varied within uncertainty for each simulation: the flight path distance, TOF zero time, experimental data points, and background normalization factors. The transmissions for each sample were then input into SAMMY along with relevant SAMMY input fitting parameters: effective temperature, sample thicknesses, burst width, resolution function parameters, energy range of SAMMY fit, and the order of the samples in the sequential SAMMY calculation. Each of the listed inputs were randomly sampled within their uncertainties from their probability distributions during the analysis: flight path (Gaussian), TOF zero time (Gaussian), magnitude of each experimental data point (Gaussian), background normalization factors (uniform), effective temperature (Gaussian), sample thicknesses (Gaussian), burst width (Gaussian), resolution function parameters (uniform), energy range of SAMMY fit (uniform), and the order of the samples in the sequential SAMMY calculation (uniform).

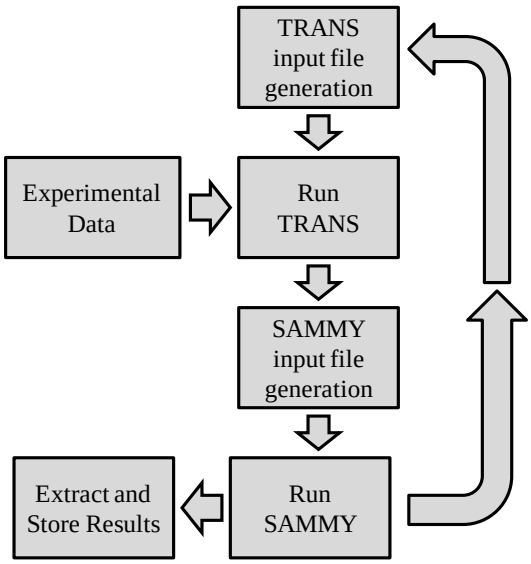

Figure 2. Diagram depicting the sequence of steps in the Monte Carlo uncertainty propagation method.

The program provides an output vector, r_i, for each relevant SAMMY output (energy, Γ_γ, Γ_n, normalization). The final result is the mean of the output vectors, $\bar{r}$, and the uncertainty is reported as the standard deviation, $\overline{\sigma_r}$,as shown in Equations (4) and (5).

$$\bar{r} = \frac{1}{n}\sum_{i=1}^{n} r_i \tag{4}$$

$$\overline{\sigma_r} = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(r_i - \bar{r})^2} \tag{5}$$

3. RESULTS AND DISCUSSION

The TMC method employed using the SAMMY code yielded resonance parameters for the 5.47 eV resonance in ^{236}U. Table I shows how the Monte Carlo method results compare to those of running SAMMY alone for single sets of input parameters. The Local, Midway, and Distant refer to the background normalization used: Local and Distant being the bounding local and distant background information and Midway being halfway between those bounding values. These bounding values show how great the affect of the background normalization is on the resulting resonance parameters. Table I also shows the difference propagating non-linear effects with the Monte Carlo method has on the magnitude of the uncertainty on the resonance parameters, with the uncertainty on Γ_γ doubling in value and Γ_n increasing by a factor of 5.

Table I. Comparison of Monte Carlo Results with Individual SAMMY simulations

Input Parameters	Energy [eV]	Γ_γ [meV]	Γ_n [meV]
Local	5.4677±0.0001	28.7±0.5	2.143±0.008
Midway	5.4672±0.0001	26.5±0.5	2.131±0.008
Distant	5.4667±0.0001	24.4±0.5	2.135±0.007
Monte Carlo	5.467±0.005	27±1	2.13±0.04

Table II shows how the Monte Carlo (RPI) results compare with other published evaluated data. This table shows the difference in resonance parameter data among the different evaluations, particularly Γ_n. It also shows that the Monte Carlo results are reasonable in value, essentially agreeing with the Mughabghab [9] evaluation within uncertainties.

Table II. Comparison of Monte Carlo Results with Established Evaluations

Evaluation	Energy [eV]	Γ_γ [meV]	Γ_n [meV]
ENDF-7.1 [5]	5.45	24.5	2.24
JEFF-3.2 [7]	5.45	24.5	2.16
JENDL-4.0 [8]	5.456	24.5	2.30
Mughabghab [9]	5.45±0.03	24.7±0.6	2.19±0.08
Monte Carlo (RPI)	**5.467±0.005**	**27±1**	**2.13±0.04**

4. CONCLUSION

A Monte Carlo method was employed that simulated the data reduction to transmission along with the Bayesian analysis code SAMMY to extract resonance parameters for multiple simulations. The simulations were compiled and analyzed to report resonance parameters that fit the 5.47 eV resonance in

^{236}U as well as the appropriate uncertainties on those parameters. The uncertainties reported include propagation of all relevant input uncertainties, including non-linear effects, giving the best possible estimation of the uncertainty.

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