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In the United States, the Evaluated Nuclear Data File (ENDF) system [1] is the repository for evaluated cross-section data. For resonance isotopes in neutron cross-section evaluations, the unresolved-resonance region (URR) is an energy region in which the experimental resolution is inadequate for determining the resonance parameters of individual resonances. Energy-averaged unresolved-resonance parameters are typically provided for the URR, and the resonance parameters are averages of resolved-resonance parameters over specific energy intervals. Due to the statistical nature of the unresolved-resonance parameters, probability tables can be used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the URR. Different approaches can be used to generate probability tables for an isotope of interest. The historical approach is to generate continuous-energy cross-section data from a "ladder" of resonances and determine contributions to a probability table based on the point data [2]. A new and different procedure relative to the "ladder" approach is used in the AMPX [3] cross-section processing system that has been developed at the Oak Ridge National Laboratory (ORNL). A new AMPX module, PURM (**P**robability tables for the **U**nresolved **R**egion using **M**onte Carlo), has been developed to calculate probability tables in the URR using Monte Carlo (MC) procedures. The purpose of this work is to present the MC-based approach for calculating probability tables in the URR.

In the Monte Carlo approach used in AMPX, probability tables are calculated on an ENDF evaluator-defined energy grid in the URR. For each probability table, pairs of resonances surrounding the reference energy are sampled from a Wigner spacing distribution [4]. The resonance distribution is sampled for each spin sequence (i.e., ℓ, J pair), and the number of resonances to sample for each spin sequence is determined by using the Δ_3-statistics test [5, 6]. For each resonance, the resonance widths are sampled from a Chi-square (χ^2) distribution for a specified number of degrees of freedom. Once the resonance parameters are sampled, the total, capture, fission and scatter cross sections are calculated at the reference energy using the single-level Breit-Wigner formalism with appropriate treatment for temperature effects. The cross-section calculation constitutes a single iteration or history. For the cross-section calculation and corresponding probability-table calculation, a user-specified number of batches with a corresponding number of histories per batch is processed. For each history, the total, capture, fission and scatter cross sections are calculated at the reference energy, and the corresponding contribution to the probability table is determined for each history. After completing the specified number of histories for a batch, a batch estimate for the probability for each cross-section band within a table is obtained by dividing the number of tallies for the band by the total number of histories processed. Additional batches are processed until the user-specified number of batches are complete. Additional details of the Monte Carlo procedures will be provided in the full paper. Due to the statistical nature of the calculational procedures, the PURM module provides a mechanism for monitoring the convergence of the cross-section calculation. For each reaction, a plot of the calculated cross section is provided as a function of the number of batches that are processed. Additional statistical checks are provided for each cross-section calculation (e.g., Chi-square test for normality, frequency distribution plots, etc.).

In order to demonstrate the calculation procedures, PURM has been used to calculate probability tables for ENDF/B-6 ^{235}U (MAT = 9228) in the URR. For ENDF/B-6 ^{235}U, the URR extends from 2.25 keV to

25 keV, and the evaluation has 14 reference energies in the unresolved region. PURM was used to calculate 14 probability tables that correspond to the reference energies in the evaluation. Each probability table was calculated at 300 K using 200 batches with 50 histories per batch for a total of 10,000 histories per table. The PURM results for the probability table, which is based on the total cross section, at 2.25 keV are presented in Figure 1. For ^{235}U, the probability tables were calculated with 5 nonequal probable cross-section bands. In Figure 1, the lower and upper band limits for the first band are 11.86 barns (b) and 15.30 barns, respectively. The upper limits for cross-section bands 2 through 5 are 18.97 b, 23.51 b, 29.15 b, and 56.28 b, respectively. The PURM-generated probability tables for ^{235}U were also compared with probability tables generated using the NJOY module PURR [7]. The NJOY results for ^{235}U are also presented in Figure 1. The probability tables and cross-section values that were calculated by PURM are within 2 standard deviations of the NJOY results. Similar agreement has been observed between PURM and NJOY for the remaining 13 probability tables that were calculated for ^{235}U. The verification studies with NJOY establish the computational capability for generating probability tables using Monte Carlo procedures.

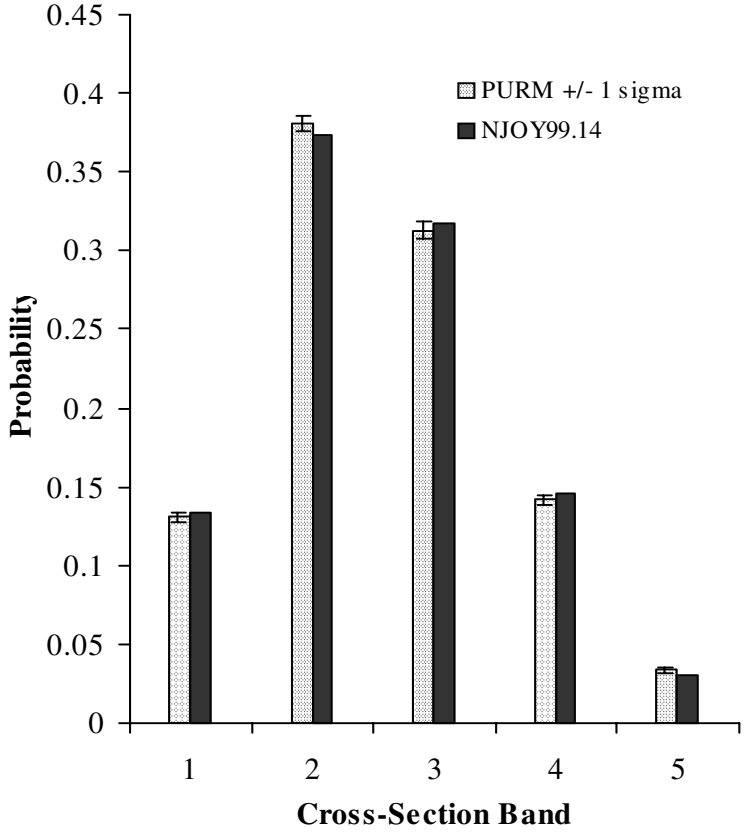

Figure 1: Probability-table comparison between PURM and NJOY for ^{235}U at 2.25 keV and 300 K.

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